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REDUCTIONS OF THE SPIN-ROTOR HAMILTONIAN

by

Maria Villa Villa

(C)

A THESIS

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Quien hubiera dicho
que estos poemas de otros
iban a ser mios
despues de todo hay hombres que no fui
y sin embargo quise ser
en cambio hay hombres que fui
y ya no soy ni puedo ser

Mario Benedetti

Abstract

The A and the S reduced Hamiltonians were used for the fitting of the rotational spectra arising from molecules with an unpaired electron. In this thesis the rotor and the spin-rotor Hamiltonians are expressed as vectors in multidimensional operator spaces. The reduction of the Hamiltonian, and the transformation between two different reduced Hamiltonians, are expressed as rotations of the Hamiltonian.

Two main points are being studied. The first involves the behavior of the two reductions with respect to: a) the asymmetry of the rotor, and b) the tendency in the molecule towards an A reduction. The study was based upon the quality of the fitting obtained. Because experimental spectra for molecules with variations in the parameters under study are not available, artificial spectra were generated.

The strong dependence of the A reduction on the asymmetry of the molecule is shown. This is in agreement with previous results reported in the literature. The results also show that the presence of an A tendency is an important feature in determining the usefulness of the A reduction. In the absence of an A tendency, the S reduction is superior.

The second main point involves the transformation between two spin-rotor Hamiltonians connected by a rotation, with the requirement that at least the rotated Hamiltonian be reduced. It is shown that the rotor part is not changed

in the spin-rotor transformation so that it is valid to focus upon the spin-rotor problem alone. The method of invariant combinations was initially used for obtaining the transformation. An invariant combination is a function of the parameters in the Hamiltonian which is invariant under a rotation.

A new method, called the rotation method in this thesis, was also developed. This method not only provides a connection between two spin-rotor Hamiltonians, but also permits the determination of the parameters in the rotation operator.

The comparative quality of the fittings obtained with two reduced Hamiltonians is related to the order of magnitude of the parameters in the rotation operator. The orders of magnitude of the parameters in the rotation operator used for a reduction give a measure of the orders of magnitude of the parameters obtained with the corresponding reduced Hamiltonian.

Finally, the A and the S reductions are used to fit the NH_2 spectrum, which is the only one available in sufficient extent and precision to satisfy the requirements of the model Hamiltonian used in this thesis. The results are in agreement with the studies done with artificial spectra.

One can relate the information obtained by artificial spectra to real molecules provided as much experimental information as possible is used in the generation of the artificial spectra.

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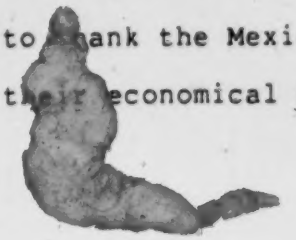

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I. INTRODUCTION

The purpose of this work is to study certain aspects of the rotational Hamiltonian of molecules with an unpaired electron. The presence of an unpaired electron doubles the lines in the rotational spectrum of the molecule through the interaction between the electronic spin and molecular rotation. The Hamiltonian reflects this in being divisible into rotor and spin-rotor parts. The development of the latter part, which is of primary interest in this thesis, was given by Van Vleck[1] in 1952. The whole Hamiltonian is written as a sum of individual terms, each consisting of an angular momentum operator and a numerical parameter (or constant) whose value depends upon the molecular system and state under consideration. The operators in the rotor part refer to molecular rotation whereas those in the spin-rotor part are products of rotor and spin angular momenta.

An important part of the analysis of experimental data is the numerical determination of values of the parameters of the Hamiltonian in order to reproduce the experimental spectrum of a specific molecular system and state. This is usually done by a least squares fitting to the spectrum. Although the process of fitting is quite simple, it turns out that the spin-rotor constants derived by Van Vleck are linearly dependent so that not all can be obtained from an experimental spectrum.

The same problem was treated by Watson[2-4] in the case of the rotor Hamiltonian. The method of contact

transformations was used, in order to eliminate the linear dependences among the parameters in the Hamiltonian. Once these are removed, the process of fitting can be carried out.

A contact transformation is the operator analogue of a unitary transformation in matrix theory. Just as the eigenvalues of a matrix are unchanged in the process, so a contact transformation does not change the eigenvalues of the Hamiltonian. Therefore, the transformed Hamiltonian is an equally valid basis for fitting an experimental spectrum. The transformation operator contained within the contact transformation is also written as a sum of terms which are products of a numerical constant and an angular momentum operator. The values of the constants are completely arbitrary, i.e., the Hamiltonian obtained from fitting a spectrum is not unique and depends on the values given to the constants in the transformation operator. The non-unique solution to the problem reflects the linear dependence mentioned above. The number of linear dependences is equal to the number of parameters in the transformation operator. These are restricted in number and once a specific set of values is chosen, the linear dependences of the Hamiltonian parameters are removed.

Although the linear dependences can be resolved in an *ad hoc* way by setting certain constants to zero, the contact transformation method has the advantage of a firm theoretical basis for such action.

The physical model used for the rotor Hamiltonian is studied in Chapter II of this thesis. Although the rotor part is not the principal consideration of this thesis, the chapter introduces concepts which are of use in studying both parts of the Hamiltonian.

One of these concepts is the classification of the parameters on the basis of order of magnitude and the parallel truncation of the Hamiltonian and transformation operators according to the precision required by the experimental data available. It should be noted that 'magnitude' is used in this thesis in a sense opposite to that more frequently found. The principal rotor constants, which are related to the moments of inertia of the molecule, are taken to be of zeroth magnitude. The principal spin-rotor constants, which are approximately a factor of 10^2 smaller in size, are taken to be of second magnitude. Thus the phrase 'higher order of magnitude' indicates a smaller size.

The major concept introduced in Chapter II is the treatment of the Hamiltonian and transformation operators as vectors in multidimensional vector spaces. The individual angular momentum operators are regarded as the basis vectors in such a space and the composite Hamiltonian and transformation operators are therefore vectors with components given by the parameters multiplying each individual angular momentum operator.

The vector representation shows that the contact transformation procedure can be expressed as a rotation to the Hamiltonian. This approach is different from those used before in the mathematical treatment of the contact transformation method. As a consequence, the connection between two sets of parameters corresponding to the same eigenvalue problem can be expressed as a rotation operator.

The number of parameters in the transformation operator (dimension of the corresponding operator space) specifies the degrees of freedom in the rotation to the Hamiltonian. As mentioned above, this is also related to the number of linear dependences among the parameters in the Hamiltonian. The elimination of the linear dependences, by applying a specific rotation to the Hamiltonian, is equivalent to assigning specific values to a certain number of parameters in the transformed Hamiltonian. For convenience, the numerical value is chosen to be zero since the parameters in the contact transformation (rotation) operator are arbitrary in any case. The result of the contact transformation is a reduced Hamiltonian (smaller number of parameters) which has zero components upon a certain number of axes in the operator-vector space for the Hamiltonian.

The dimensions of the vector spaces used in both cases are also discussed. Special emphasis is placed upon the case where the operators are truncated beyond tenth order of magnitude. Tenth order of magnitude is in agreement with the experimental results presently available.

There are two advantages to the use of the concepts of vector spaces and the representation of the contact transformations as rotations in the space of the Hamiltonian. One is the simplicity of thought and expression permitted by the ideas. The other is the parallel simplicity of the mathematical equations required.

There are many ways for obtaining a reduced Hamiltonian, but the most commonly used schemes are the A and the S reductions, introduced by Watson[5] and Winnewisser[6]. The A reduction was selected for convenience in the diagonalization of the Hamiltonian matrix because the A reduced matrix has a codiagonal structure. The S reduction was selected for the case of a near symmetric rotor, where the A reduction failed.

The physical model for the spin-rotor Hamiltonian is studied in Chapter III. The Hamiltonian and the transformation operators are expressed as vectors in a similar way to the rotor case. This assists in pointing out similarities between the rotor and the spin-rotor case. The order of magnitude separation and the dimensions of the operator spaces are also studied.

The rotor Hamiltonian parameters are shown to be mathematically invariant under the spin-rotor transformation. One can say that, with the spin-rotor transformation operator, the only Hamiltonian that is rotated is the spin-rotor Hamiltonian. With the rotor transformation operator, the whole Hamiltonian (rotor and

spin-rotor part) is rotated. This fact is fundamental to the study undertaken here. One can safely assume that the rotor reduction has been completely carried out before considering the effect of the spin-rotor reduction and that no further changes in the rotor Hamiltonian are possible as a consequence of the latter reduction.

Brown and Sears[7] have done the transformation of the spin-rotor Hamiltonian truncated at fourth degree operators. In this thesis the same case is considered but with a truncation beyond sixth degree operators. The A and the S reduction schemes for the spin-rotor Hamiltonian, introduced by Brown and Sears[7], are discussed. It is shown that the A spin-rotor reduction is not unique. The ambiguity first appears in the sixth degree operators and was therefore not previously noted.

In order to fit a spectrum, one must choose a certain scheme of reduction. The choice is primarily made on the basis of the quality of the fitting that can be obtained. It is therefore important to make a comparative study of the different schemes of reduction available for the spin-rotor in order to have criteria for the selection of a reduction in the fitting procedure. Thus the remainder of the thesis concentrates on the comparison of the non-reduced, the A reduced and the S reduced spin-rotor Hamiltonians.

A specific reduced spin-rotor Hamiltonian can be obtained by a fitting. It is convenient to have a set of equations that relates the parameters of two different

reduced Hamltonians. In that case, one does not have to do a second fitting to the spectrum in order to assess other reduced Hamiltonians. Instead one has only to solve such a set of equations.

Birss et al.[8] have used the method of invariant combinations for obtaining the transformation between two different reduced rotor Hamiltonians. In Chapter IV this method is analysed. As defined by these authors, an invariant combination is a linear combination of coefficients, or products of coefficients, which has an identical value within any reduction of the Hamiltonian. In Chapter IV the combinations are defined in terms of invariance under a rotation of the Hamitonian and this concept is developed into a method of deriving them.

The invariant combinations for the case of the spin-rotor Hamiltonian are discussed in Chapter V. These explicit numerical forms are proven to be invariant under a rotation and linearly independent. Unfortunately, the method of invariant combinations is not practical for this particular case because of their complexity. As a consequence, the solution to the invariant combination equations does not have the required numerical precision. Therefore this method, which was the approach initially proposed for the subject of this thesis, was abandoned.

A second method is proposed in Chapter IV which is called the rotation method because it involves the explicit determination of the parameters in the rotation (contact

transformation) operator. Using the formalism developed in Chapter III, the rotation to the Hamiltonian is expressed in terms of a transformation matrix which depends upon the parameters in the rotation operator. This is developed into a set of equations in which the parameters of the reduced Hamiltonian are expressed as functions of the rotation parameters and those of the original Hamiltonian. This set is then used for two purposes. Those equations involving parameters which are zero in the reduced spin-rotor Hamiltonian are used to determine the parameters of the rotation. These are then substituted into the remaining equations to give the values of the parameters in the rotated (reduced) Hamiltonian.

In an initial comparison of the invariant combination and rotation methods, the former appears to be better. It provides a single set of equations which can be used for the connection among all reductions whereas the rotation method is explicitly dependent upon the two reductions under consideration. The initial reason for abandoning the invariant combination method was the difficulties with numerical precision, which are not encountered in the rotation method. However, the rotation method has a byproduct which is so useful that would in any case lead to it being the preferred method. This byproduct is the explicit values of the transformation parameters.

The rotation method can be used to connect two different reduced Hamiltonians, one of which is the result

of a fitting to experimental data. If the quality of the fitting is good, the values of the rotation parameters give a measure of the quality of the fitting that can be expected with the second Hamiltonian. Further, the departure of the rotation parameters from the theoretical orders of magnitude is reflected in the corresponding distortion of the magnitudes of the parameters in the second reduction.

An example of the dependence mentioned above is that given by Winnewisser[6] in the rotor case. The molecule he studied is DSSD which is accidentally very nearly a symmetric rotor. The values of the parameters involved in the rotation for obtaining the A reduction are severely distorted in terms of order of magnitude. This distortion is reflected in the parameters of the A reduced Hamiltonian, and does not allow the fitting procedure to have the required precision. Indeed, the case is so extreme that a fitting in the A reduction does not converge.

Another case where the rotation method can be applied is in the transformation of a non-reduced to a reduced Hamiltonian. That can, of course, be done only in the hypothetical case where the parameters of the non-reduced Hamiltonian are available.

The rotation method is applied to the A and S reductions of the spin-rotor Hamiltonian in Chapter VI. It is important to make a comparative study of the behavior of reductions with respect to variations in the Hamiltonian parameters of the molecule whose spectrum is to be fitted.

With that kind of study, one can develop a firm basis for the selection of a reduction scheme. This is the ultimate purpose of the thesis.

The first parameter to be studied is the K (asymmetry) parameter which measures the departure from the symmetric rotor condition. Experimental spectra for molecules with different values of asymmetry are not available to the precision required by the model used in this work. The only adequate experimental information is for the NH_2 molecule, with a value of K equal to -0.4, corresponding to a quite highly asymmetric rotor. Hypothetical values for the Hamiltonian constants are therefore given in order to obtain artificial spectra of molecules with different values of K. To make the artificial spectra reasonably simulate real cases, the information available for the NH_2 is extrapolated to other K. Two main characteristics are taken into account for the spectra generation: the ratio between the principal constants in the rotor and the spin-rotor Hamiltonians is maintained at the NH_2 value; idealized orders of magnitude of the higher degree rotor and spin-rotor constants are used.

The other parameter that is varied during the spectra production is the presence of an A tendency in the molecule. The A tendency is produced by giving to the parameters eliminated in an A reduction smaller values than specified by the idealized classification.

In Chapter VI, the behavior of the A and the S reductions is studied with respect to variations in the two parameters mentioned above. The tables given in that chapter contain the values of the standard deviations obtained in the fittings of reduced Hamitonians to the artificial spectra generated with a non-reduced Hamiltonian. The standard deviation is taken as a measure of the quality of the fitting.

Three different kinds of studies are done:

1) Rotor and spin-rotor reduction. Four different schemes of reduction are investigated: A-A', A-S', S-S', and S-A', i.e., all possible mixtures of reduction between the rotor and spin-rotor parts of the Hamiltonian.

2) Spin-rotor reduction. The rotor part is not reduced and the fitting procedure is done in two different ways: a) the rotor parameters are varied in the fitting procedure, and b) the rotor parameters remain constant, with only the spin-rotor part varied in the fitting.

3) Rotor reduction. The rotor reduction is done without reducing the spin-rotor part. The influence of the extent of the spin-rotor part during the rotor reduction is also studied. This particular pattern of investigation was, in part, undertaken in order to demonstrate the essential independence of the rotor and spin-rotor parts of the Hamiltonian with respect to behavior under reductions.

The conclusions arrived at are:

1) The parameter K influences the A reduction in both the rotor and the spin-rotor parts. The smaller the asymmetry of the molecule, the bigger the value of the standard deviation obtained by the A reduction. The quality of the fitting with an S reduction is reasonably stable with respect to changes in the value of K.

2) The existence of an A tendency in a molecule improves the quality of the fitting in both schemes of reduction. The A reduction is, of course, more sensitive to this parameter than the S reduction.

3) The S reduction gives a better fitting unless the molecule has a pronounced A tendency. The influence of asymmetry had been recognized since the work of Winnewisser[8], but the additional effect of an A tendency had not previously been noted.

4) The first step during a fitting procedure should be the variation of the rotor parameters. Once the rotor part is adjusted to give a reasonably low value in the standard deviation, the spin-rotor part is varied. When the spin-rotor parameters are introduced, the rotor parameters must also be varied because there is significant correlation between the two sets.

The generation of artificial spectra provides the opportunity of 'knowing' the non-reduced Hamiltonian. By the use of the rotation method one can obtain the values of the parameters in the reduction operator. One can also compare the values of the Hamiltonian parameters obtained by the

rotation method and those obtained by the fitting procedure.

This comparison gives rise to the conclusions:

1) The order of magnitude of the parameters in the reduction operator is also a measure of the quality of the fitting obtained by the reduced Hamiltonian. Any distortion in the orders of magnitude of the reduction operator is reflected in the standard deviation of the fitting.

2) Any magnitude distortion in the parameters of the reduction operator is also reflected in the magnitudes of the parameters of the Hamiltonian.

3) If there is no distortion in the reduction operator, Hamiltonians obtained by the two methods are in reasonable agreement so that the proposed values in the generated reduction serve as an excellent starting point for fitting.

4) Although the use of the rotation method is theoretically legitimate only when the rotor parameters remain unchanged between reductions, the above considerations are empirically found to apply when the rotor parameters are varied within a fitting and consequently differ substantially between reductions. This broadens the applicability of the present study to cover real as well as artificial cases.

When the rotation method is used for transformation between reductions, the above conclusions, which are based upon the non-reduced to reduced transformation, are found to apply. This completes the applicability to real cases because fittings to experimental spectra can only be carried

out within a reduction.

Finally, a fitting to the experimental NH_2 spectrum[9-17] is done in two stages:

1) The spectrum is truncated beyond N=10, in order to follow the characteristics used in the artifical spectra generation. The A and the S fittings give essentially the same standard deviation. Since the S reduction contains some of the constants which are eliminated in the A reduction, the presence of an A tendency is clearly detectable. This is in agreement with the conclusions obtained from the artificial spectra which again shows that the study of artificial spectra can be applied to experimental situations. One should be very careful to use as much experimental information as possible in order to produce artificial spectra that reasonably simulate real cases.

2) The fitting of the full NH_2 spectrum (3500 items of data) was then done, using as a starting point the reduced Hamiltonians obtained from the fittings to the truncated spectrum.

II. ROTOR HAMILTONIAN

A. ROTOR HAMILTONIAN MODEL

In the analysis of the motion of a molecule there are various approximations which must be made in order to obtain a Hamiltonian that is useful for the fitting of spectra. One assumes the separability of the electronic and nuclear motions, due to their differences in masses and velocity. The nuclear motion can also be separated approximately into three different kinds of motion: translational, vibrational and rotational. As a result the Hamiltonian for a molecule in which the translational motion is neglected can be written as

$$H = H(e) + H(v) + H(r) \ , \qquad \text{(II.1)}$$

where $H(e)$, $H(v)$ and $H(r)$ are the electronic, vibrational and rotational Hamiltonians. The purpose of the present chapter is the study of the rotational motion.

Generally the Hamiltonian is written within the concept of a molecular frame and principal moments of inertia. The molecular frame is a set of Cartesian coordinates which rotates with the molecule with its origin located at the center of mass of the molecule.

The most general rotational Hamiltonian is that of an asymmetric rotor:

$$H = \Sigma_{x1,x2}\, h_{x1,x2}\, N_{x1}N_{x2} \qquad \text{(II.2)}$$

where x1,x2 = x,y,z and the N_{x_i} are the dimensionless angular momentum operators: N_x, N_y, N_z. The constants $h_{x1,x2}$

$$h_{x1,x2} = h^2/8\pi^2 I_{x1,x2} \qquad \text{(II.3)}$$

are functions of the elements of the inertia tensor ($I_{x1,x2}$), with h in h^2 being Planck's constant. Equation (II.2) will be called the reference Hamiltonian. The concept of principal moments of inertia is the result of the diagonalization of the inertia tensor to obtain:

$$H = h_{x,x}N_x^2 + h_{y,y}N_y^2 + h_{z,z}N_z^2. \qquad \text{(II.4)}$$

This procedure is discussed in detail in section C of this chapter. Throughout this thesis, operators are represented as italic characters.

At the same time that the molecule is rotating, vibrations are taking place. The moments of inertia are functions of the normal coordinates of vibration. The constants $h_{x1,x2}$ can be expanded in a Taylor series about the equilibrium position in terms of the normal coordinates of vibration, q_i. The expansion truncated up to first order terms can be written as:[18]

$$h_{x1,x2} = h^{o}_{x1,x2} + \Sigma_i \, (\partial h_{x1,x2}/\partial q_i)^{o} \, q_i \qquad \text{(II.5)}$$

where the superscript zero indicates evaluation at the equilibrium position. The Hamiltonian corresponding to the distortion produced by the vibration is:

$$H' = \Sigma_{x1,x2} \, [\, \Sigma_i \, (\partial h_{x1,x2}/\partial q_i)^{o} q_i \,] N_{x1} N_{x2} \, . \qquad \text{(II.6)}$$

Using second order perturbation theory, the Hamiltonian can be written:

$$H = \Sigma_{x1,x2} \, h^{o}_{x1,x2} \, N_{x1} N_{x2}$$
$$+ \Sigma_{x1,x2,x3,x4} \, (\, h_{x1,x2,x3,x4} \, N_{x1} N_{x2} N_{x3} N_{x4} \,) \, . \qquad \text{(II.7)}$$

In equation (II.7) there is no explicit dependence on the vibrational operator so that it corresponds to the Hamiltonian associated with a single vibrational state. The constants depend upon the vibrational frequencies, ω_i [19,20]:

$$h_{x1,x2,x3,x4} = -h^{6} \Sigma_i \, (\partial I_{x1,x2}/\partial q_i)^{o} \, (\partial I_{x3,x4}/\partial q_i)^{o}$$
$$\cdot (1/2h^{3}c^{3}\omega_i^{2} \, I_{x1,x1} I_{x2,x2} I_{x3,x3} I_{x4,x4}) . \qquad \text{(II.8)}$$

These h's are called centrifugal distortion constants. If the perturbation method is carried on to higher orders , the final Hamiltonian will be expressed in terms of operators containing even powers of angular momentum operators. Because the additional terms in the reference Hamiltonian

arise from the use of perturbation theory, the Hamiltonian can be partitioned in terms of orders of magnitude of the coefficients (as well as degree of angular momentum operators).

$$H = H^{0,2} + H^{4,4} + H^{8,6} + \ldots \qquad \text{(II.9)}$$

indicating with the first superscript the order of magnitude associated with the coefficients, and with the second the degree of the operators. This can be written as

$$H = \Sigma_n H^{2n-4,n} \qquad \text{(II.10)}$$

where:

$$H^{2n-4,n} = \Sigma_{x1,x2\ldots xn} (h^{2n-4}_{x1,x2\ldots xn} N_{x1} N_{x2} \ldots N_{xn}) \qquad \text{(II.11)}$$

and x1,x2...xn correspond to x,y,z. In equation (II.11) the nth degree Hamiltonian is expressed as a sum of operators of a certain degree (n), multiplied by coefficients of a specific order of magnitude (2n-4). The order of magnitude is related to the degree so that, from now on, only the superscript corresponding to the degree will be associated with the Hamiltonian.

The commutation relations among the angular momentum operators with respect to the rotating frame are

$$[N_{x1} , N_{x2}] = -iN_{x3}, \qquad (II.12)$$

where x1,x2,x3 form an even permutation of x,y,z. Using these one can simplify the Hamiltonian and write it in what is called in the literature[2] the standard form

$$H = \Sigma_n \Sigma_{i,j,k} h^{2n}_{i,j,k} \{ N_x^i N_y^j N_z^k \} \qquad (II.13)$$

with i+j+k=n. The operator in braces is an hermitian operator

$$\{ N_x^i N_y^j N_z^k \} = N_x^i N_y^j N_z^k + N_z^k N_y^j N_x^i \qquad (II.14)$$

and i+j+k is even.

The Hamiltonian has to satisfy two physical requirements: hermiticity and invariance with respect to time reversal (Θ) . Each operator in the Hamiltonian behaves in the following way under such operations:

$$N_{xi}\dagger = N_{xi} \qquad (II.15)$$

$$\Theta N_{xi} \Theta^{-1} = - N_{xi}, \qquad (II.16)$$

where $\dagger$ is used for expressing the adjoint, so that

$$\{ N_x^i N_y^j N_z^k \}\dagger = \{ N_x^i N_y^j N_z^k \} \qquad (II.17)$$

$$\Theta\{ N_x^{\,i}\, N_y^{\,j}\, N_z^{\,k} \}\Theta^{-1} = \{ N_x^{\,i}\, N_y^{\,j}\, N_z^{\,k} \} \ . \qquad \text{(II.18)}$$

Equation (II.18) takes into consideration that i+j+k is an even number. In order for the Hamiltonian to satisfy the hermiticity and the invariance with respect to time reversal, the constants within it must be real.

Each set of values {i,j,k} corresponds to a unique operator and coefficient. In order to make the nomenclature clearer, one can assign a single index to the second sum in equation (II.13),

$$H = \Sigma_n \Sigma_m \, h_m^{2n-4} \, O_m^n \ . \qquad \text{(II.19)},$$

In equation (II.19), the following definition has been used:

$$O_m = \{ N_x^{\,i(m)}\, N_y^{\,j(m)}\, N_z^{\,k(m)} \} \ , \qquad \text{(II.20)}$$

where the m is associated with i, j and k to emphasize a specific set of values. Table II.1 clarifies the definition in equation (II.20) for the second degree operators.

Table II.1

ROTOR HAMILTONIAN OPERATORS

O_m	m	i(m)	j(m)	k(m)
N_x^2	1	2	0	0
$\{ N_x N_y \}$	2	1	1	0
$\{ N_x N_z \}$	3	1	0	1
N_y^2	4	0	2	0
$\{ N_y N_z \}$	5	0	1	1
N_z^2	6	0	0	2

Equation (II.19) may be reinterpreted in terms of vectors in a multidimensional space. The operators O_m^n are regarded as unit vectors, $\mathbf{O}_m^n$, serving as basis for the space. The Hamiltonian is therefore a vector expressed in this basis. This is written as

$$\mathbf{H} = \Sigma_n \Sigma_i \mathbf{O}_i^n \, h_i^{2n-4} = \mathbf{Oh} \qquad \text{(II.21)}$$

in which **O** is the collection of basis vectors, $\mathbf{O}_i^n$, viewed as a row vector and **h** is the collection of coefficients, h_i^{2n-4}, viewed as a column vector. From now on, boldface characters are used to represent both vectors in a multidimensional space ($\mathbf{O}_i^n$, **H**) and vectors in the matrix sense (**O**, **h**).

In order to describe the vector space introduced in equation (II.21), one defines its dimensions. For this purpose it is better to divide the Hamiltonian into

subspaces according to degree of angular momentum operators (order of magnitude of the coefficients), as in equation (II.10).

If n is equal to the degree of the operator, in terms of angular momentum operators, and d(n) is the dimension of the space, one can write:

$$H^n = \Sigma_{i=1}^{d(n)} h_i^{2n-4} O_i^n \qquad \text{(II.22)}$$

$$d(n) = (1/2)(n+1)(n+2) \qquad \text{(II.23)}$$

$$\mathbf{H}^n = \mathbf{O}^n \mathbf{h}^{2n-4} \ . \qquad \text{(II.24)}$$

This is not the only basis in which the Hamiltonian can be written. If one wants to use another operator basis (linear combinations of the standard one), the relationship can be expressed as a matrix transformation. For representing matrices, bold characters will be used in the same way as for vectors. A vector space O_1 in basis 1 is related to its representation in basis 2, O_2, by

$$\mathbf{O}_1 = \mathbf{O}_2 \mathbf{T}_{2,1} \qquad \text{(II.25)}$$

where $\mathbf{T}_{2,1}$ is the matrix transformation from basis 2 to basis 1. Since

$$H = O_1\, h_1 = O_2\, h_2 \qquad \text{(II.26)}$$

and, from equation (II.25):

$$H = O_2\, T_{2,1}\, h_1 \qquad \text{(II.27)}$$

one obtains:

$$h_2 = T_{2,1}\, h_1 \ . \qquad \text{(II.28)}$$

Aside from the standard form, the most commonly used basis in the literature is the one consisting of combinations of the following operators:

$$N^2 = N_x^2 + N_y^2 + N_z^2 \qquad \text{(II.29)}$$

$$N_z^2 = N_z^2 \qquad \text{(II.30)}$$

$$f^k = N_+^k + N_-^k \ . \qquad \text{(II.31)}$$

Because of its characteristics, this basis will be called the ladder basis.

Some constraints have to be imposed on the Hamiltonian for practical requirements:

1) The order of magnitude of the coefficients associated with operators of degree n is $2n-4^2$.

2) It will not be useful to express the Hamiltonian in terms of a vector space of infinite dimension. Using the concept of order of magnitude of the coefficients, one can truncate the Hamiltonian at the precision required by the experimental data available. In this work, the truncation will be done at tenth order of magnitude.

As a conclusion, the following table can be written:

TABLE II.2

ROTOR HAMILTONIÁN VECTOR SPACE DIMENSIONS

degree of operator	order of magnitude	dimension of space
2	0	6
4	4	15
6	8	28

B. UNITARY TRANSFORMATION AS A ROTATION TO THE HAMILTONIAN

The solution to the Schrödinger equation involving the rotor Hamiltonian is written as an eigenvalue equation

$$H\psi_i = E_i\psi_i \ . \qquad \text{(II.32)}$$

A unitary operator U which has the property

$$U\dagger = U^{-1} , \tag{II.33}$$

can be used to transform the Hamiltonian according to

$$H' = U\dagger H U . \tag{II.34}$$

This form is called a contact transformation.

The eigenvalues of the original Hamiltonian remain unchanged under a contact transformation. This statement can be proved by applying the unitary operator to equation (II.32):

$$U\dagger H \psi_i = E_i U\dagger \psi_i . \tag{II.35}$$

Inserting the unit operator in the form $U U\dagger$, one obtains

$$U\dagger H U U\dagger \psi_i = E_i U\dagger \psi_i , \tag{II.36}$$

and, from equation (II.34),

$$H' (U\dagger \psi_i) = E_i (U\dagger \psi_i). \tag{II.37}$$

Therefore, although one applies a contact transformation to the Hamiltonian, one is still dealing with the eigenvalues of the original problem.

The unitary operator U can be expressed in terms of a transformation operator T by

$$U = \exp(+i\, T) \; . \qquad \text{(II.38)}$$

This has the form of a rotational transformation operator so that the contact transformation to the Hamiltonian may be viewed as a rotation of the Hamiltonian. This will be discussed later, after obtaining a specific expression for the transformation operator.

The adjoint of equation (II.38) is:

$$U\dagger = \exp(-i\, T\dagger) \; . \qquad \text{(II.39)}$$

In order for U to be unitary, the transformation operator T must be hermitian

$$T\dagger = T \; . \qquad \text{(II.40)}$$

Using equations (II.39) and (II.40):

$$U\dagger\, U = \exp(-i\, T) \exp(+i\, T) \qquad \text{(II.41)}$$

$$U\dagger\, U = 1 \; . \qquad \text{(II.42)}$$

For the analysis of the transformation operator it is convenient to write the unitary operator as a Taylor expansion:

$$U = 1 + iT - (1/2)T^2 + \ldots \qquad \text{(II.43)}$$

Substituting equation (II.43) into equation (II.34) one obtains the transformed Hamiltonian H'

$$H' = H - i[T,H] - (1/2)[T,[T,H]] + \ldots \qquad \text{(II.44)}$$

in terms of commutators between the original one and the transformation operator.

The Hamiltonian must remain hermitian and invariant under time reversal after the contact transformation. One must determine the restrictions on the transformation operator in order to satisfy the requirements mentioned above. For mathematical simplicity, equation (II.44) can be truncated at first order terms, and the adjoint can be written as:

$$H'\dagger = H\dagger + i[T,H]\dagger \ . \qquad \text{(II.45)}$$

Because the adjoint reverses the order of products, this is

$$H'\dagger = H\dagger - i[T\dagger,H\dagger] \ . \qquad \text{(II.46)}$$

The original Hamiltonian and the transformation operator are hermitian so that

$$H'\dagger = H - i[T,H] \tag{II.47}$$

and

$$H'\dagger = H' \tag{II.48}$$

i.e., the transformed Hamiltonian is already hermitian because of the hermitian nature of H and T.

Applying the time reversal operator θ to equation (II.44) one obtains

$$\Theta H'\Theta^{-1} = \Theta H\Theta^{-1} + i[\ \Theta T\Theta^{-1}\ ,\ \Theta H\Theta^{-1}\ ]. \tag{II.49}$$

The original Hamiltonian is invariant under time reversal, so that:

$$\Theta H'\Theta^{-1} = H + i[\ \Theta T\Theta^{-1}\ ,\ H\ ]\ . \tag{II.50}$$

For the transformed Hamiltonian to be invariant under time reversal, the transformation operator must change sign under time reversal

$$\Theta\ T\ \Theta^{-1} = -\ T\ , \tag{II.51}$$

since, substituting equation (II.51) into equation (II.50), one obtains

$$\Theta H' \Theta^{-1} = H - i[\, T \,,\, H \,] \,, \qquad \text{(II.52)}$$

which leads to

$$\Theta \, H' \, \Theta^{-1} = H' . \qquad \text{(II.53)}$$

To proceed further one must study the transformation operator in terms of the Hamiltonian to which it is going to be applied, that is, the rotational Hamiltonian. From equation (II.19):

$$H = \Sigma_n \, \Sigma_{i=1}^{q(n)} \, h_i^{2n-q} \, O_{2,i}^n \,. \qquad \text{(II.54)}$$

A subindex, 2, is associated with the operator O in order to specify that the sum over n includes only even numbers.

We want the transformed Hamiltonian to be expressed in the same space as the untransformed one. The transformed Hamiltonian is written in terms of nested commutators of the operator T and the original Hamiltonian. Because of the commutation relations among the angular momentum operators, equation (II.12), the transformation operator must be written in terms of a power series of angular momentum operators, in order to remain in the same space after the transformation:

$$T = \Sigma_n \, \Sigma_{i=1}^{q(n)} \, t_i \, O_i^n \qquad \text{(II.55)}$$

where d(n) is given by equation (II.23) and the t_i's are a set of constants.

There are some physical restrictions which must be imposed on the transformation operator:

T must be hermitian. The adjoint of the transformation operator is

$$T\dagger = \Sigma_n \Sigma_{i=1}^{d(n)} t_i^* O_i^n\dagger \ . \qquad \text{(II.56)}$$

From the definition of O_i^n, and from equation (II.17),

$$O_i^n\dagger = O_i^n \ . \qquad \text{(II.57)}$$

From equation (II.57), equation (II.56) can be written as

$$T\dagger = \Sigma_n \Sigma_{i=1}^{d(n)} t_i^* O_i^n \ . \qquad \text{(II.58)}$$

In order for T to be hermitian, the constants must be real

$$t_i = t_i^* \ . \qquad \text{(II.59)}$$

From equation (II.51), T must change sign under time reversal. From equation (II.55)

$$\Theta T \Theta^{-1} = \Sigma_n \Sigma_{i=1}^{d(n)} t_i^* \Theta O_i^n \Theta^{-1} \ , \qquad \text{(II.60)}$$

and, from equation (II.16),

$$\Theta O_1^n \Theta^{-1} = (-1)^n O_1^n \quad . \tag{II.61}$$

Substitution of equation (II.61) into equation (II.60) yields

$$\Theta T \Theta^{-1} = \Sigma_n \, (-1)^n \, \Sigma_{i=1}^{d(n)} \, t_i \, O_1^n \quad . \tag{II.62}$$

In order to satisfy equation (II.51), the sum over n must be restricted to odd integers. By analogy to the notation used in the Hamiltonian, the O's within the transformation operator will have a subscript of 1, to denote that only odd n terms are included.

The orders of magnitude of the coefficients in T must be determined. For that purpose one can substitute equation (II.54), with n equal to odd numbers only, and equation (II.55) into equation (II.44) and, by truncation up to first order terms, obtain:

$$H' = \Sigma_n \, \Sigma_{i=1}^{d(n)} \, h_i^{2n-4} O_{2,i}^n$$
$$-i[\Sigma_n \, \Sigma_{j=1}^{d(n)} \, t_j O_{1,j}^n \, , \, \Sigma_{i=1}^{6} \, h_i^0 O_{2,i}^2] \quad . \tag{II.63}$$

In equation (II.63), the Hamiltonian written in the commutator has been truncated up to zeroth order of magnitude terms so that one obtains only the leading terms with respect to order of magnitude considerations. The specific commutators occurring in equation (II.63) are exposed by reordering the summations as

$$H' = \Sigma_n \Sigma_{i=1}^{d(n)} h_i^{2n-4} O_{2,i}^n$$
$$-i \Sigma_{i=1}^{6} \{ \Sigma_n \Sigma_{j=1}^{d(n)} h_i^0 t_j [O_{1,j}^n , O_{2,i}^2] \}. \quad (II.64)$$

The commutation relations of the angular momentum operators, equation (II.12), allows one to represent the commutators in terms of matrices c_j of coefficients defined by

$$- i[O_{1,j}^n , O_{2,i}^2] = \Sigma_{k=1}^{d(n+1)} c_j(k,i) O_{2,k}^{n+1} . \quad (II.65)$$

Once again, one considers only the terms of the commutator that contribute to operators of n+1 degree, which are the leading ones in terms of order of magnitude considerations.

From equation (II.64), the terms that will be introduced by the contact transformation, to operators of n+1 degree, can be written by using equation (II.65) as:

$$-i[t_j O_{1,j}^n , O_2^2 h^0] = t_j O_2^{n+1} c_j h^0 \quad (II.66)$$

where matrix and vector notation has been used. The order of magnitude of the coefficent t_j in the transformation operator corresponding to operators of degree n must equal the order of magnitude of the coefficients of n+1 degree in the Hamiltonian, i.e., 2n-2. Therefore, the transformation operator can be written as

$$T = \Sigma_n \Sigma_{i=1}^{d(n)} t_i^{2n-2} O_{1,i}^n , \quad (II.67)$$

or in vector representation,

$$T = O_1 \, t \, . \tag{II.68}$$

The superscript 2n-2 on t_j^{2n-2} simply denotes the order of magnitude of the t coefficients.

The transformation operator, like the Hamiltonian, is a vector in a multidimensional operator space. The transformation operator , and the operator space, can also be partitioned in terms of degree of operators as well as order of magnitude of the coefficients as follows:

$$T = \Sigma_n \, T^n = \Sigma_n \, O_i^n \, t^{2n-2} \, . \tag{II.69}$$

The only difference between the vector spaces for the Hamiltonian and for the transformation operators is that the Hamiltonian is constrained to an even degree operator space and the transformation vector to one of odd degree. In a similar way, for the reasons mentioned above, the transformation operator will be truncated for the purposes of this work at tenth order of magnitude. The dimensions of the vector space are given in Table II.3.

TABLE II.3

TRANSFORMATION VECTOR SPACE DIMENSIONS

degree of operator	order of magnitude	dimension of space
1	0	3
3	4	10
5	8	21

Equation (II.34), in vector notation, is

$$\mathbf{H}' = \exp(-i\mathbf{O}_1 t)\, \mathbf{H}\, \exp(i\mathbf{O}_1 t) \ . \qquad \text{(II.70)}$$

Here, the view that the contact transformation is a rotation of the Hamiltonian is specified clearly. In order to emphasize that the transformation operator is used for a rotation of the Hamiltonian, it will henceforth be called the rotation operator. The rotation and the Hamiltonian are operators, but are most easily discussed in terms of their vector representation in an operator space. One can use the operator or the vector representation according to mathematical convenience.

Equation (II.70) can be written as

$$\mathbf{H}' = \exp(-i\mathbf{O}_1 t)\, \mathbf{O}_2 \mathbf{h}\, \exp(+i\mathbf{O}_1 t) \ . \qquad \text{(II.71)}$$

After a Taylor expansion of the exponential operators, one

obtains

$$H' = \Sigma_j \, ((-i)^j/j!) \, [\, O_1 t \, , \, O_2 h \,]^{(j)} \, , \qquad \text{(II.72)}$$

where (j) indicates the order of nesting of the commutator in terms of the rotation operator, i.e.,

$$H' = H - i \, [\, O_1 t \, , \, O_2 h \,] - (1/2) \, [\, O_1 t \, , \, [\, O_1 t \, , \, O_2 h \,] \,] + \ldots \, . \qquad \text{(II.73)}$$

One can combine equations (II.70), (II.71) and (II.73) into an exponential form:

$$H' = \exp(-i[\, O_1 t \, , \, * \,]) \, O_2 h \qquad \text{(II.74)}$$

$$H' = \exp(-i[\, T \, , \, * \,]) \, H \, . \qquad \text{(II.75)}$$

The asterisk indicates the position that the following operator is to occupy when the exponents are developed as in equation (II.73).

Equation (II.75) is a very useful equation because of its mathematical simplicity. In the following sections the mathematical advantages of expressing the rotation to the Hamiltonian as an exponential commutator operator will become clear.

C. DETERMINABILITY OF THE PARAMETERS IN THE HAMILTONIAN

The experimental data that one can obtain from molecular rotation are contained in a spectrum. As a result of the analysis of such a spectrum, one can obtain the experimental eigenvalues (or differences in eigenvalues) of the Hamiltonian for the molecule. A model Hamiltonian was proposed in Section II.A. Its eigenvalues may be determined by diagonalization of its matrix representation in an appropiate basis of functions f_k . In matrix form equation (II.22) is:

$$\mathbf{H} = \Sigma_n \Sigma_{i=1}^{d(n)} \mathbf{O}_{2,i}^n \, h_i^{2n-4}, \qquad \text{(II.76)}$$

with matrix elements:

$$\mathbf{H}_{k,m} = \langle f_k \mid H \mid f_m \rangle , \qquad \text{(II.77)}$$

$$(\mathbf{O}_{2,i}^n)_{k,m} = \langle f_k \mid O_{2,i}^n \mid f_m \rangle . \qquad \text{(II.78)}$$

For practical purposes, equation (II.76) has three main characteristics:

1) The Hamiltonian is written in terms of operators whose matrix elements can be calculated easily.

2) The problem of obtaining the Hamiltonian for a given molecule is restricted now to determining an appropriate set of values for the constants contained in the Hamiltonian model. To get a good set of constants means to be able to

reproduce the eigenvalues or differences in eigenvalues that were obtained from the experimental spectrum. This procedure is called a fitting to the spectrum.

3) An experimental spectrum is always restricted by precision considerations. The rotational Hamiltonian in equation (II.76) is divided in terms of order of magnitude of its coefficients. The foregoing property makes it possible to truncate the Hamiltonian at the terms of order of magnitude that are in agreement with the precision of the experimental data available.

From the preceding section, one can write the Hamiltonian after the rotation in the following way

$$H' = \Sigma_n \Sigma_{i=1}^{d(n)} O_{2,i}^n h_i^{2n-4'}. \qquad \text{(II.79)}$$

The rotation operator does not change the eigenvalues of the Hamiltonian, inside the order of magnitude considerations. The sets of constants h_i and h_i' from equations (II.76) and (II.79) are equivalent solutions to the experimental spectrum. The Hamiltonian is not unique, and this gives rise to indeterminability of the coefficients in the Hamiltonian.

If one considers only an nth degree Hamiltonian, and truncates the expansion of the rotation operator at linear terms of the proper order of magnitude, one can write

$$O_2^n h^{2n-4'} = O_2^n h^{2n-4} - i \left[O_1^{n-1} t^{2n-4} , O_2^2 h^0 \right] . \qquad \text{(II.80)}$$

Using operator notation for the transformation vector, one obtains:

$$O_2^n h^{2n-4'} = O_2^n h^{2n-4} - i \Sigma_{j=1}^{d(n-1)} t_j^{2n-4} [O_1^n , O_2^2 h^0]. \quad \text{(II.81)}$$

From equation (II.64), one obtains

$$-i [O_1^n , O_2^2 h^0] = \Sigma_{k=1}^{s} -i [O_1^n , O_{2,k}^2] h_k^0, \quad \text{(II.82)}$$

and

$$-i [O_1^n , O_2^2 h^0] = \Sigma_{k=1}^{s} \Sigma_{m=1}^{d(n)} O_{2,m}^n c_j(m,k) h_k^0. \quad \text{(II.83)}$$

One can arrange the $c_j(m,k)$ elements in a matrix array which allows equation (II.83) to be written as

$$-i [O_1^n , O_2^2 h^0] = O_2^n c_j h^0 . \quad \text{(II.84)}$$

If one defines

$$c_j h^0 = c_j^0 , \quad \text{(II.85)}$$

and

$$-i\,[\,O_1^n\,,\,O_2^2 h^0\,] = O_2^n\,c_j^0, \qquad \text{(II.86)}$$

then, upon substituting (II.86) into (II.81), one obtains

$$O_2^n\,h^{2n-4'} = O_2^n\,h^{2n-4} + \Sigma_{j=1}^{d(n-1)}\,O_2^n\,t_j^{2n-4}\,c_j^0 \qquad \text{(II.87)}$$

$$O_2^n\,h^{2n-4'} = O_2^n\,(\,h^{2n-4} + \Sigma_{j=1}^{d(n-1)}\,t_j^{2n-4}\,c_j^0\,)\,. \qquad \text{(II.88)}$$

Thus, from equation (II.88), one obtains:

$$h^{2n-4'} = h^{2n-4} + \Sigma_{j=1}^{d(n-1)}\,t_j^{2n-4}\,c_j^0\,. \qquad \text{(II.89)}$$

This is a system of d(n) linear equations with more variables, the d(n) h^{2n-4} and d(n-1) t^{2n-4}, than equations. Equation (II.89) is the mathematical expression for the absence of a unique solution to the rotational Hamiltonian. In order to be able to solve the system, one has to give arbitrary values to d(n-1) variables. The dimension of the space for the rotation operator is the number of degrees of freedom to which arbitrary values for the constants in the Hamiltonian may be assigned. It can be taken as the number of linear dependences among the constants.

One has to give arbitrary values to d(n-1) variables, in order to eliminate the linear dependences among the nth degree Hamiltonian constants, and then proceed to the fitting procedure for that degree. The simplest choice for the arbitrary value to be given is zero. Thinking of the

Hamiltonian as a vector, the assignment of zero value to a certain number of constants corresponds to a specific rotation of the original Hamiltonian. As a consequence , the nth degree Hamiltonian to be used for the fitting procedure will contain only (n+1) variables since, from equation (II.23)

$$d(n) - d(n-1) = (1/2)\{(n+1)(n+2)-n(n+1)\}$$

$$= n + 1 . \qquad \text{(II.90)}$$

The Hamiltonian to be fitted will be a reduced Hamiltonian and the rotation operator becomes a reduction operator. Following the scheme used in sections A and B of this chapter, the truncation of the Hamiltonian up to tenth order of magnitude results in the dimensionalities given in Table II.4.

TABLE II.4

DIMENSIONS OF ROTOR VECTOR SPACE

order of magnitude	original Hamitonian	rotation operator	reduced Hamiltonian
0	6	3	3
4	15	10	5
8	28	21	7

One can divide the reduction procedure into two steps: first the reduction of the zeroth order of magnitude Hamiltonian, and subsequently the reduction of the remaining part.

The zeroth order of magnitude Hamiltionian

$$H^0 = \Sigma_{i=1}^{6} h_i^0 O_{2,i}^2 \qquad \text{(II.91)}$$

is reduced by the rotation operator

$$T^0 = \Sigma_{i=1}^{3} t_i^0 O_{1,i}^2 \, . \qquad \text{(II.92)}$$

The rotation cannot usefully be expressed as a Taylor expansion. The truncation of the expansion is not valid because the zero order of magnitude of the coefficients does not allow the series to converge. The T^0 operator has instead the advantage of being a rotation in the physical three dimensional angular momentum space. The coefficients h^0 are the components of the inertia tensor, $\mathbf{h}^0$. Using $\mathbf{N}$ to represent the vector $[\, N_x \;\; N_y \;\; N_z \,]$, the zero order Hamiltonian is

$$\mathbf{H} = \mathbf{N}\, \mathbf{h}^0\, \mathbf{N}\dagger . \qquad \text{(II.93)}$$

Three coefficients of $\mathbf{h}$ may be made equal to zero. The three remaining non-zero coefficients are the principal moments of inertia, that is, the rotation operator of equation (II.92)

may be used to diagonalize the inertia tensor

$$\begin{vmatrix} h_{xx} & 0 & 0 \\ 0 & h_{yy} & 0 \\ 0 & 0 & h_{zz} \end{vmatrix} . \qquad \text{(II.94)}$$

The final result is the rotational Hamiltonian referred to in equation (II.3):

$$H^{0\prime} = h^0_{xx}N_x^2 + h^0_{yy}N_y^2 + h^0_{zz}N_z^2 . \qquad \text{(II.95)}$$

When the zeroth order of magnitude reduction is done, the higher order of magnitude terms are also changed because the rotation is applied to the whole Hamiltonian.

The starting point for the higher order of magnitude reductions is the Hamiltonian obtained after the zeroth order reduction. The reduction can be done in two steps: the orthorhombic symmetry reduction and what will be called the ladder basis reduction.

In the symmetry reduction the orthorhombic point group is chosen in order to be consistent with the zeroth order of magnitude Hamiltonian expressed in equation (II.95), which belongs to the orthorhombic group. Watson[2] has proven that the number of nth order of magnitude Hamiltonian operators belonging to the non-totally symmetric representation of the orthorhombic point group are the same in the Hamiltonian and in the rotation operator. Therefore, the coefficients in the

Hamiltonian corresponding to operators that do not belong to the totally symmetric representation of the orthorhombic point group, can be made equal to zero by those in the rotation operator that also do not belong to the totally symmetric representation. The former reduction can be called a symmetry reduction because, as a consequence of it, one is left with a Hamiltonian and a rotation operator that correspond to a molecule with an orthorhombic symmetry.

The operators in the symmetry reduced Hamiltonian are of the form:

$$O_2^n = \{ N_x^i N_y^j N_z^k \} , \qquad \text{(II.96)}$$

where i,j,k are even numbers. The operators in the symmetry reduced rotation operator are:

$$O_1^n = \{ N_x^i N_y^j N_z^k \} , \qquad \text{(II.97)}$$

where i,j,k are odd numbers. The dimensions of the various spaces associated with the symmetry reduction and the subsequent ladder reduction are given in Tables II.5 and II.6.

TABLE II.5

DIMENSIONS FOR THE SYMMETRY REDUCTION

order of magnitude	non-reduced Hamiltonian	symmetry rotation operator	symmetry reduced Hamiltonian
0	6	3	3
4	15	9	6
8	28	18	10

TABLE II.6

DIMENSIONS FOR THE LADDER REDUCTION

order of magnitude	symmetry reduced Hamiltonian	ladder rotation operator	reduced Hamiltonian
0	3	0	3
4	6	1	5
8	10	3	7

The last part of the reduction is called the ladder reduction because it is based upon the reduction of the Hamiltonian expressed in the ladder operator basis. This is the most convenient for recognizing the matrix elements corresponding to a certain O_2^0 operator.

There are many different ways in which the Hamiltonian can be reduced, which may be called schemes of reduction.

There are two main schemes that are most commonly used in the literature[5,6]. They are called the asymmetric (A) reduction, and the symmetric (S) reduction. The asymmetric reduction consists of giving the value zero to the coefficients in the reduced Hamiltonian which correspond to operators with matrix elements in a symmetric rotor basis $|N,k\rangle$:

$$\langle N, k \mid O_2^n \mid N, k\pm\Delta k \rangle \neq 0 \ , \ \Delta k > 2 \ . \qquad \text{(II.98)}$$

In other words, the coefficients corresponding to operators

$$O_2^n = \{ N^i N_z^j f^k \} \ , \ k > 2 \qquad \text{(II.99)}$$

are put to zero in the A reduced Hamiltonian. From equation (II.98) the matrix representation of the A reduced Hamiltonian is a codiagonal matrix

$$\langle N, k \mid H \mid N, k\pm\Delta k \rangle = 0 \ , \ \Delta k > 2 \ , \qquad \text{(II.100)}$$

and is therefore very convenient for diagonalization purposes. Winnewisser[6] and Watson[5] have shown that the A reduction does not work when the molecule is a near symmetric rotor. The concept of order of magnitude of the parameters in the rotation operator is destroyed when differences between pairs of the principal moments of inertia are very small.

Winnewisser[8] has introduced the S reduction, which consists of putting to zero those coefficients corresponding to operators containing the N_z operator with non-diagonal matrix elements. In other words, the coefficients corresponding to operators

$$O_2^n = [\, N^i \, N_z^j \,] \, , \, [\, N^i \, f^k \,] \qquad \text{(II.101)}$$

are those with non-zero coefficients in the S reduced Hamiltonian. The S reduction is more general because it can be applied to any kind of molecule.

III. SPIN-ROTOR HAMILTONIAN

A. SPIN-ROTOR HAMILTONIAN MODEL

It was assumed above that the motion of the nuclei is independent of the motion of the electrons. This section considers the interaction of the rotational motion of the nuclei and the spin angular momentum of the electrons, more often called spin-rotation interaction. The simplest case in which the interaction takes place is when there is a single unpaired electron, which arises in molecules in a doublet electronic state.

The nuclei are electric charges in motion, and they create an electric field[21]. The electric field created by a nucleus of charge $Z_k e$ at the position of the electron is

$$E_k = (Z_k e)\ (R_k)^{-3}\ (R_k)\ . \qquad \text{(III.1)}$$

The vector R_k refers to the position of the electron with respect to the kth nucleus. The magnetic field experienced by the electron as a consequence of the electric field in equation (III.1) is:

$$M_k = E_k \times (\ (1/2)v(e) - v_k\ ) / c \qquad \text{(III.2)}$$

where $[\ (1/2)v(e) - v_k\ ]$ is the effective velocity of the electron relative to that of the nucleus and c is the speed of light. Substituting equation (III.1) into (III.2), and

summing over all the nuclei, the total magnetic field is:

$$\mathbf{M} = \Sigma_k \, [\, Z_k \, e \, R_k^{-3} \, \mathbf{R}_k \times (\, (1/2)\mathbf{v}(e) - \mathbf{v}_k \,) \, / \, c \,] . \quad \text{(III.3)}$$

The energy of interaction between the magnetic moment of the electron and the magnetic field of the nuclei is[21]

$$H(\text{int}) = -\mathbf{M} \cdot \mu(e) \quad \text{(III.4)}$$

where $\mu(e)$ is the magnetic moment of the unpaired electron. In terms of spin dimensionless angular momentum, S, it can be defined as[22]

$$\mu(e) = - \, (eh/2\pi mc) \, \mathbf{S} \quad \text{(III.5)}$$

where e is the charge of the electron and m is the electron mass. Substitution of equations (III.3) and (III.5) into equation (III.4) gives

$$H(\text{int}) = (eh/2\pi mc^2) \, \Sigma_k \, Z_k e R_k^{-3} \cdot [\, \mathbf{R}_k \times (\, (1/2)\mathbf{v}(e) - \mathbf{v}_k \,) \,] \cdot \mathbf{S} \, . \quad \text{(III.6)}$$

The energy of interaction, $H(\text{int})$, can be divided into two parts, one containing nuclear velocities as factors, and the other containing the electron velocity. The latter term is:

$$H(e) = (eh/4\pi mc^2)\ \Sigma_k\ Z_k e R_k^{-3}\ \{R_k \times v(e)\} \cdot S. \qquad (III.7)$$

Van Vleck[1] has shown that $H(e)$ can be written in terms of linear combinations of double products of spin angular momentum operators. For the case of one unpaired electron (doublet state), the $H(e)$ term is a constant contribution to the energy, and can be included in the band origin.

The energy term containing the nuclear velocities is:

$$H(s\text{-}r) = -(eh/2\pi mc^2)\ \Sigma_k\ Z_k e R_k^{-3}\ \{R_k \times v_k\} \cdot S. \qquad (III.8)$$

Further development of this form is possible with the definitions

$$v_k = \omega \times r_k \qquad (III.9)$$

$$\omega_{xi} = N_{xi}/I_{xi,xi} \qquad (III.10)$$

where ω is the angular velocity of the molecule, with components ω_{xi}, $I_{xi,xi}$ is the instantaneous moment of inertia about axis xi, and r_k is the distance between the nucleus k and the center of mass. The xi specify the Cartesian axes in the rotating molecular frame to which the components of S are also referred. Using these substitutions, the component in S_x of equation (III.8) is:

$$H(s\text{-}r,S_x) = \Sigma_k\ p_k\ P_{k,x}\ S_x \qquad \text{(III.11)}$$

where:

$$p_k = -\ (\ Z_k e^2 h\ )/(\ 2\pi mc^2 R_k^3\ ) \qquad \text{(III.12)}$$

and

$$P_{k,x} = \{\ \mathbf{R}_k \times \omega \times \mathbf{r}_k\ \}_x \qquad \text{(III.13)}$$

Developing the cross products and using equation (III.10), this is

$$P_{k,x} = (R_{k,y}r_{k,y} + R_{k,z}r_{k,z})\ (N_x/I_x) - R_{k,y}r_{k,x}(N_y/I_y) - R_{k,z}r_{k,x}(N_z/I_z) \qquad \text{(III.14)}$$

Substitution of equation (III.14) into equation (III.11) gives:

$$H(s\text{-}r,S_x) = \Sigma_k\ (hp_k/2\pi)\ \{\ (R_{k,y}r_{k,y} + R_{k,z}r_{k,z})\ (N_xS_x)/I_x - (R_{k,y}r_{k,x})\ (N_yS_x)/I_y - (R_{k,z}r_{k,x})\ (N_zS_x)/I_z\ \} \qquad \text{(III.15)}$$

Doing the same thing for the y and z components, one obtains the equation for the spin-rotor Hamiltonian that is commonly used in the literature

$$H(s\text{-}r) = \Sigma_{x1,x2}\, h^{s}_{x1,x2}\, N_{x1}\, S_{x2} \qquad \text{(III.16)}$$

The $h^{s}_{x1,x2}$ constants depend on the x1 instantanous moments of inertia and, following Raynes[22], are defined by:

$$h^{s}_{x1,x1} = \Sigma_k\, (hp_k/2\pi I_{x1})(R_{k,x2}r_{k,x2} + R_{k,x3}r_{k,x3}) \qquad \text{(III.17)}$$

$$h^{s}_{x1,x2} = -\Sigma_k\, (hp_k/2\pi I_{x1})\, (\, R_{k,x1}r_{k,x2}\,)\, . \qquad \text{(III.18)}$$

The reference Hamiltonian including the rotor part and the spin-rotor interactions is now

$$H = \Sigma_{x1}\, h^{o}_{x1,x1}N_{x1}^{2} + \Sigma_{x1,x2}\, h^{s}_{x1,x2}N_{x1}S_{x2} \qquad \text{(III.19)}$$

where the coefficients in the spin-rotor interaction, $h^{s}_{x1,x2}$, are of second order of magnitude with respect to the $h^{o}_{x1,x1}$ coefficients. The interaction with the vibrations can now be considered, following the procedure used in the previous chapter. The $h^{s}_{x1,x2}$ coefficients are expanded in a Taylor series in terms of the normal coordinates of vibration[18] and perturbation theory for a single electronic and vibrational state is carried out. The final Hamiltonian can be divided into a pure rotor part and a spin-rotor part. The pure rotor part is the one obtained previously in equation (II.19). The spin-rotor part is the one to be studied here. It consists of linear combinations of

operators containing angular momentum operators of different degrees

$$H(s\text{-}r) = \Sigma_n \Sigma_{i=1}^{q(n)} h_i^n O_i^n \qquad \text{(III.20)}$$

where:

$$O_m^n = \{ N_x^{i(m)} N_y^{j(m)} N_z^{k(m)} S_{x1(m)} \} \qquad \text{(III.21)}$$

$$\{ N_x^{i(m)} N_y^{j(m)} N_z^{k(m)} S_{x1(m)} \} = N_x^{i(m)} N_y^{j(m)} N_z^{k(m)} S_{x1(m)} + S_{x1(m)} N_z^{k(m)} N_y^{j(m)} N_{x(m)}^{i} \qquad \text{(III.22)}$$

with x1(m) = x, y or z and n = i(m)+j(m)+k(m). The m has been introduced in equations (III.21) and (III.22) in order to emphasize that in equation (III.20) a single index was associated with a particular coefficient-operator pair. Operators containing spin operators higher than first degree do not arise in the case of a doublet state. It was mentioned before that such higher order terms can be taken as a constant contribution to the energy of the system. All the operators arising from permutations of the elements of the operator in equation (III.21) can be eliminated by the use of the commutation relations among the angular momentum operators in the molecular frame[23]:

$$[N_{x1} , N_{x2}] = -i N_{x3} \qquad \text{(III.23)}$$

$$[N_{x1} , S_{x2}] = -i S_{x3} \qquad \text{(III.24)}$$

$$[S_{x1} , S_{x2}] = -i S_{x3} \qquad \text{(III.25)}$$

where x1,x2,x3 is an even permutation of x,y,z.

The spin-rotor Hamiltonian must be hermitian:

$$H(s\text{-}r) = H(s\text{-}r)\dagger \ . \qquad \text{(III.26)}$$

From equation (III.20)

$$H(s\text{-}r)\dagger = \Sigma_n \Sigma_{i=1}^{q(n)} h_i^* O_{i\cdot n}\dagger . \qquad \text{(III.27)}$$

Since

$$S_{xj}\dagger = S_{xj} \qquad \text{(III.28)}$$

and the N_{xj} are self-adjoint (equation (II.17)),

$$O_{i\cdot n}\dagger = O_{i\cdot n} \ . \qquad \text{(III.29)}$$

Therefore

$$H(s\text{-}r)\dagger = \Sigma_n \Sigma_{i=1}^{q(n)} h_i^* O_{i\cdot n} \ , \qquad \text{(III.30)}$$

and, in order for the spin-rotor Hamiltonian to be hermitian, the constants have to be real.

The spin-rotor Hamiltonian must also be invariant under time reversal

$$\Theta H(s\text{-}r)\Theta^{-1} = H(s\text{-}r) \ . \qquad \text{(III.31)}$$

From equation (III.25),

$$\Theta H(s\text{-}r)\Theta^{-1} = \Sigma_n \Sigma^{q(n)}_{i=1} h^i_* \Theta O^i_{1\cdots n}\Theta^{-1} \ . \qquad \text{(III.32)}$$

But, from equation (III.17), and

$$\Theta S_{x\,i}\Theta^{-1} = -S_{x\,i}, \qquad \text{(III.33)}$$

it follows:

$$\Theta O^i_{1\cdots n}\Theta^{-1} = (-1)^{n+1} O^i_{1\cdots n}. \qquad \text{(III.34)}$$

Using equations (III.31) and (III.34) in equation (III.32):

$$\Theta H\Theta^{-1} = \Sigma_n (-1)^{n+1}\Sigma^{q(n)}_{i=1} h^i_* O^i_{1\cdots n} \qquad \text{(III.35)}$$

In order for the spin-rotor Hamiltonian to be invariant under time reversal, the sum over n must include only odd numbers. Following the same nomenclature that was used for the operators in the rotor Hamiltonian, the spin-rotor

Hamiltonian can be written as

$$H(s\text{-}r) = \Sigma_n \Sigma_{i=1}^{d(n)} h_i^{\dagger} O_i^{\dagger} \qquad \text{(III.36)}$$

with

$$d(n) = (3/2)\,(n+1)\,(n+2)\,. \qquad \text{(III.37)}$$

In general, the order of magnitude of the spin-rotor coefficient $h_i^{\dagger}$ associated with the operator $O_i^{\dagger}$ is 2n, so it is useful to denote this coefficient as $h_i^{\dagger\,2n}$ to show its order of magnitude explicitly.

In the same way as the rotor Hamiltonian, the spin-rotor Hamiltonian can be written as a vector in a multidimensional operator space:

$$H(s\text{-}r) = O_i^{\dagger}\, h^{\dagger} = \Sigma_n O_i^{\dagger\,n}\, h^{\dagger\,2n} \qquad \text{(III.38)}$$

and can also be subdivided in terms of order of magnitude or degree of rotational angular momentum operators. The dimensions of the operator vector spaces for the spin-rotor Hamiltonian to tenth order of magnitude are given in Table II.1.

TABLE III.1

DIMENSIONS FOR THE SPIN-ROTOR HAMILTONIAN

order of magnitude	degree of operator	dimension of space
2	1	9
6	3	30
10	5	63

The standard form of equation (III.21) is not the only one that is commonly used. The ladder form is constructed using the following operators as a basis

$$\mathbf{N}\cdot\mathbf{S} = N_x S_x + N_y S_y + N_z S_z \qquad \text{(III.39)}$$

$$N_z S_z \qquad \text{(III.40)}$$

$$f^k F = N_+ {}^k S_+ + N_- {}^k S_- \qquad \text{(III.41)}$$

in analogy with equations (II.29), (II.30) and (II.31) for the rotor case. The spin rotor Hamiltonian in this basis can be written in the form of equation (II.39), but the operators $O_i^{(n)}$ and the coefficients $h^{(2n)}$ necessarily differ from those in the Cartesian basis.

B. ROTATION OF THE SPIN-ROTOR HAMILTONIAN

The total Hamiltonian will be the sum of the rotor and the spin-rotor part:

$$H = H(r) + H(s\text{-}r) \; . \tag{III.42}$$

By applying a contact transformation to the Hamiltonian one obtains

$$H' = \exp(-i[T,*])\, H \; . \tag{III.43}$$

In a similar way to the Hamiltonian, the transformation operator can be divided into a rotor and a spin-rotor part:

$$T = T(r) + T(s\text{-}r) \; . \tag{III.44}$$

The rotation to the Hamiltonian can therefore also be divided into steps:

$$H'' = \exp(-i[T(s\text{-}r),*])\, \exp(-i[T(r),*])\, H. \tag{III.45}$$

An intermediate transformed Hamiltonian

$$H' = \exp(-i[T(r),*])\, H(r) + \exp(-i[T(r),*])\, H(s\text{-}r) \tag{III.46}$$

is obtained after the rotor rotation. The effect of the

rotor rotation on the rotor Hamiltonian has been described in detail in Chapter II, and one has now to study its effect on the spin-rotor Hamiltonian:

$$H'(s\text{-}r) = \exp(-i[T(r),*])\, H(s\text{-}r) \; . \qquad \text{(III.47)}$$

Expressing the exponential operator as a Taylor expansion truncated at first order terms, one obtains:

$$H'(s\text{-}r) = H(s\text{-}r) - i[\, T(r) \, , \, H(s\text{-}r)] \; . \qquad \text{(III.48)}$$

In lowest order (see equation (II.68) and Table II.6) $T(r)$ consists of the single term $t^1_1 \; O^3_{1,1}$. Substituting the Hamiltonian from equation (III.36), one obtains:

$$H(s\text{-}r)' = H(s\text{-}r) + \Sigma_n \; \Sigma^{(n)}_{\lambda;\mu} \; \{ \; -i[\; t^1_1 \; O^3_{1,1} \; , \; h^{1\cdot 2n}_{\lambda;\mu} \; O^{1\cdot 2n}_{\lambda;\mu}]\}. \qquad \text{(III.49)}$$

For a single value of n, and using the commutator relations in equations (III.22) to (III.24):

$$\Sigma^{(n)}_{\lambda;\mu} \; t^1_1 \; \{ \; -i[\; O^3_{1,1} \; , \; O^{1\cdot 2n}_{\lambda;\mu} \;]\} \; h^{1\cdot 2n}_{\lambda;\mu} = \Sigma^{(n)}_{\lambda;\mu} \; \Sigma^{(n\cdot 2)}_{\lambda;\mu} \; t^1_1 \; O^{1\cdot n;2}_{\lambda;\mu} \; c_1(j,i) \; h^{1\cdot 2n}_{\lambda;\mu} \qquad \text{(III.50)}$$

where $c_1(j,i)$ is defined parallel to equation (II.65). These

are the main corrections to the spin-rotor Hamiltonian of degree n+2. In vector notation the result is

$$O_i^{1,n+2}\, h^{2n+4\prime} = O_i^{1,n+2}\, h^{2n+4} + t_i^{*}\, O_i^{1,n+2}\, c_1\, h^{2n}. \qquad \text{(III.51)}$$

Equation (III.51) shows that a contact transformation, with the operator $T(r)$, applied to the spin-rotor Hamiltonian changes the values of the spin-rotor constants, depending on the t's previously chosen to effect specific changes (such as reduction) within the rotor part. Thus the intermediate Hamiltonian is:

$$H' = \Sigma_n \Sigma_i\, h_i^{2n-4\prime}\, O_{2,i}^{n} + \Sigma_n \Sigma_i\, h_i^{1,2n\prime}\, O_i^{1,n} \qquad \text{(III.52)}$$

where the limits in the sums over i are as specified above.

A second contact transformation is to be applied, with the spin-rotor transformation operator, as indicated in equation (III.45). Similar to the rotor transformation, the spin-rotor transformation operator can be written

$$T^{s} = \Sigma_n \Sigma_i^{s(n)}\, t_i^{s}\, O_i^{1,n}\ . \qquad \text{(III.53)}$$

The T^{s} operator must be hermitian:

$$T^{s} = T^{s\dagger} = \Sigma_n \Sigma_i^{s(n)}\, t_i^{s*}\, O_i^{1,n\dagger}\ . \qquad \text{(III.54)}$$

From equation (III.29), the operators in equation (III.54) are hermitian, so that

$$T'^{\dagger} = \Sigma_n \Sigma_{i,j}^{d(n)} t_i^* O_j^{1,n} . \qquad \text{(III.55)}$$

For T' to be hermitian, the constants t_i must be real. The spin-rotor transformation operator, like the rotor transformation operator, must change sign under time reversal. Since

$$\Theta T' \Theta^{-1} = \Sigma_n \Sigma_{i,j}^{d(n)} t_i^* \Theta O_j^{1,n} \Theta^{-1} , \qquad \text{(III.56)}$$

equation (III.34) and the fact that the t_i are real yield

$$\Theta T' \Theta^{-1} = \Sigma_n (-1)^{n+1} \Sigma_{i,j}^{d(n)} t_i O_j^{1,n} . \qquad \text{(III.57)}$$

In order to satisfy the change in sign under time reversal, the sum over n must be restricted to even integers, so that

$$T' = \Sigma_n \Sigma_{i,j}^{d(n)} t_i O_{2,j}^{n} . \qquad \text{(III.58)}$$

When the spin-rotor rotation is applied to the intermediate Hamiltonian of equation (III.52), one obtains

$$H'' = \exp(-i[T' , *]) (\Sigma_n \Sigma_{i,j}^{d(n)} h_i^{2n-4} O_{2,j}^{n}) + \exp(-i[T' , *]) (\Sigma_n \Sigma_{i,j}^{d(n)} h_i^{2n} O_{2,j}^{n}) . \qquad \text{(III.59)}$$

Expanding the exponential operator and truncating at first order terms, one obtains

$$H'' = H' - \Sigma_n \, i[\, T' \,,\, \Sigma_{i=1}^{q(n)} h_i^{2n-4\prime} O_{2,i}^n \,] - \Sigma_n \, i[\, T' \,,\, \Sigma_{i=1}^{q(n)} h_i^{1,2n\prime} O_{1;i}^n \,] \,. \qquad \text{(III.60)}$$

One must now analyze the changes introduced into the Hamiltonian by the spin-rotor transformation. The largest correction, in terms of order of magnitude considerations, will be the commutator of T' with the n=2 term of the rotor Hamiltonian,

$$H'' = H' - i[\, T' \,,\, \Sigma_{i=1}^{3} h_i^{0\prime} O_{2,i}^2 \,] \,. \qquad \text{(III.61)}$$

The limit on the sum over i is three because the rotational Hamiltonian is already reduced by the rotor transformation (see Table II.6). Substituting from equation (II.58), one obtains the lowest order result:

$$H'' = H' + \Sigma_n \, \Sigma_j \, \Sigma_{i=1}^{3} t_j^i \, h_i^{0\prime} \{-i[\, O_{1;j}^n \,,\, O_{2,i}^2 \,]\} \,. \qquad \text{(III.62)}$$

Consider the correction introduced by the nth degree operators of the spin-rotor transformation. Using the commutators in equations (III.22) to (III.24), the result of the commutator in equation (III.62) is an operator with one degree in spin angular momentum operators, and n+1 degrees in rotational angular momentum operators. This contributes a

change in the spin-rotor Hamiltonian but the coefficients of the rotor Hamiltonian do not change under the spin-rotor transformation. As a consequence one can concentrate upon the spin-rotor Hamiltonian. Continuing with the considerations of the nth degree spin-rotor transformation, its effect on the spin-rotor Hamiltonian is

$$H^{n+1}(s\text{-}r)'' = H^{n+1}(s\text{-}r)' + \Sigma_j \Sigma_{i=1}^{3} t_j h_i^0 \{ -i [O_{\frac{1}{2}}^{i} , O_{\frac{3}{2}}^{j}] \} . \quad \text{(III.63)}$$

As before, the commutators are expressible in terms of components of a matrix, c_j^i, defined by

$$-i[O_{\frac{1}{2}}^{i} , O_{\frac{3}{2}}^{j}] = \Sigma_k c_j^i(k,i) O_{\frac{1}{2}}^{k} \quad \text{(III.64)}$$

so that

$$H^{n+1}(s\text{-}r)'' = H^{n+1}(s\text{-}r) + \Sigma_j t_j (\Sigma_{i=1}^{3} \Sigma_k O_{\frac{1}{2}}^{k} c_j^i(k,i) h_i^0) \quad \text{(III.65)}$$

or, in vector notation

$$H^{n+1}(s\text{-}r)'' = H^{n+1}(s\text{-}r)' + \Sigma_j^{n} t_j O_{\frac{1}{2}}^{n+1} c_j h^0 . \quad \text{(III.66)}$$

Defining:

$$c_j^i \, h^{0\prime} = c_j^{i,0} \qquad \text{(III.67)}$$

one can rewrite equation (III.66) as

$$H^{n+1}(s-r)'' = H^{n+1}(s-r)' + \Sigma_{j=1}^{n} t_j^i \, O_j^{i,n+1} \, c_j^{i,0}. \qquad \text{(III.68)}$$

Two considerations should be applied to equation (III.68):

1) The coefficients t_j^i in the spin-rotor transformation associated with opertators $O_j^{i,n}$ in equation (II.78) has an order of magnitude 2n+2. It is useful to denote this coefficient as $t_j^{i,2n+2}$ to display its order of magnitude explicitly.

2) The parameters in the rotor Hamiltonian are completely independent of the spin-rotor transformation. This is a result of the properties of the commutators between rotational angular momentum and spin angular momentum, equation (III.23). It is possible to perform the rotor transformation first, and then perform the spin-rotor transformation, without affecting any of the equations for obtaining the reduced rotor Hamitonian. With the rotor transformation operator the whole Hamiltonian is rotated, whereas, with the spin-rotor transformation, only the spin-rotor part is rotated.

The spin-rotor transformation operator of equation (III.58) can be written as a vector in a multidimensional

operator space

$$T' = O_{\frac{1}{2}}^{\frac{1}{2}} t' \ . \qquad \text{(III.69)}$$

The space can be partitioned into subspaces of operators of the same degree, and one can write:

$$T' = \Sigma_n \, O_{\frac{1}{2}}^{\frac{1}{2}, n} \, t^{s, 2n+2} \ . \qquad \text{(III.70)}$$

The dimensions of the different subspaces given by equation (III.38), are shown in Table III.2 for truncation at tenth order of magnitude.

TABLE III.2

S-R TRANSFORMATION VECTOR SPACE DIMENSIONS

degree of rotational operator	order of magnitude	space dimensions
0	2	3
2	6	18
4	10	45

Analogous to the rotor transformation, there are a certain number of indeterminancies in the spin-rotor Hamiltonian parameters, corresponding to the number of linear dependences among them. The rotated spin-rotor

Hamiltonian used for a fitting procedure must be a reduced spin-rotor Hamiltonian without any indeterminancies. The reduced Hamiltonian has zero components to that number of axes (operators) equal to the dimension of the space used for the transformation operator. Different schemes of reduction can be followed, but before analysing them, some specification on the basis of molecular symmetry is required.

In the rotor case, the contact transformation was divided into two stages: the orthorhombic symmetry reduction and the ladder reduction. Regardless of the symmetry of the molecule, the orthorhombic reduction allows the reduced rotor Hamiltonian to be expressed in terms of operators which are bases to the totally symmetric representation of the largest orthorhombic group D(2h). The ladder reduction is carried out with such operators so that the symmetry of the molecule does not affect the resulting reduced Hamiltonian. In contrast, the symmetry group of the molecule determines those operators which may be included in the spin-rotor Hamiltonian and spin-rotor contact transformation operators. The origin of this is found in equation (III.8) where reference to the molecular symmetry occurs in the position of the electron with respect to the kth nucleus of the molecule, R_k. The symmetry reduction of the rotor case is therefore replaced by writing the spin-rotor Hamiltonian and contact transformation operators with individual operators constrained to be bases to the totally symmetric

representation of the symmetry group of the molecule under study. As a consequence, only the ladder reduction must be carried out.

In the case of a molecule belonging to an orthorhombic point group, which is the case to be considered in this thesis, the dimension of the nth degree spin-rotor Hamiltonian is $3(n+1)(n+3)/8$. The dimension of the nth degree spin-rotor transformation is $3(n)(n+2)/8$. As a consequence, the dimension for the nth degree reduced Hamiltonian is $3(n+1)/2$.

The truncation of the spin-rotor Hamiltonian and the spin-rotor transformation operator at tenth magnitude gives rise to the results shown in Table III.3.

TABLE III.3

SPACE DIMENSIONS FOR THE ORTHORHOMBIC SPIN-ROTOR CASE

order of magnitude	original Hamiltonian	transformation operator	reduced Hamiltonian
2	3	0	3
6	9	3	6
10	18	9	9

Among the different schemes of reduction, two have been used by Brown and Sears[7]: the A reduction and the S reduction. They obtained the spin-rotor reduced Hamiltonian from the reduced rotor Hamiltonian by replacing N^2 ,N_z^2 and

f^2, with $N\cdot S$, N_zS_z and fF. In the manner defined by Brown and Sears[7], the replacements given in Table III.4 are made.

TABLE III.4

CONSTRUCTION OF THE SPIN-ROTOR HAMILTONIAN

ROTOR HAMILTONIAN	A REDUCED SPIN-ROTOR HAMILTONIAN	S REDUCED SPIN-ROTOR HAMILTONIAN
N^2	$N\cdot S$	$N\cdot S$
N_z^2	N_zS_z	N_zS_z
f^2	fF	fF
N^4	$N^2(N\cdot S)$	$N^2(N\cdot S)$
$N^2N_z^2$	$N^2(N_zS_z)$, $N_z^2(N\cdot S)$	$N^2(N_zS_z)$, $N_z^2(N\cdot S)$
N^2f^2	$f^2(N\cdot S)$	$f^2(N\cdot S)$
N_z^4	$N_z^3S_z$	$N_z^3S_z$
$N_z^2f^2$	$f^2N_zS_z$	
f^4		f^3F
N^6	$N^4(N\cdot S)$	$N^4(N\cdot S)$
$N^4N_z^2$	$N^4(N_zS_z)$, $N^2N_z^2(N\cdot S)$	$N^4(N_zS_z)$, $N^2N_z^2(N\cdot S)$
N^4f^2	$N^2f^2(N\cdot S)$	$N^2f^2(N\cdot S)$
$N^2N_z^4$	$N^2N_z^3S_z$, $N_z^4(N\cdot S)$	$N^2N_z^3S_z$, $N_z^4(N\cdot S)$
$N^2N_z^2f^2$	$N_z^2f^2(N\cdot S)$, $N^2f^2N_zS_z$	
N^2f^4		$f^4(N\cdot S)$
$N_z^4f^2$	$f^2N_z^3S_z$	
N_z^6	$N_z^5S_z$	$N_z^5S_z$
f^6		f^5F

In the case of the S reduction, the procedure does not present any problems. However, there are ten sixth degree operators which agree with the recipe for obtaining the A reduced spin-rotor Hamiltonian but, from the Table III.3, only nine are allowed. That gives an ambiguity in the selection of the A reduced Hamiltonian at tenth order of magnitude.

This concludes the study of the rotor and spin-rotor Hamiltonians. In succeeding chapters the focus of the discussion is on the spin-rotor part. This has been shown to be feasible because the spin-rotor transformation does not alter the rotor part. It has also been shown that a specific number of coefficients in the spin-rotor Hamiltonian are indeterminate and that a reduced Hamiltonian must be used. The methods developed in the present chapter will be used to address this problem and the problem of connections between different reductions. The fundamental concept used in that study is the view of the reduction of the Hamiltonian as a rotation in a multidimensional vector space. The formalism developed on the basis of that interpretation serves as the starting point for subsequent discussions. The related definition of commutator matrices is also of fundamental importance in that work.

IV. CONNECTIONS AMONG VARIOUS SCHEMES OF REDUCTION

A. GENERAL CONSIDERATIONS

A fitting to the spectrum of a molecule must be done according to a certain scheme of reduction. There are many schemes of reduction, and therefore it is useful to be able to switch from one scheme to another, without necessarily having to do a second fitting procedure.

The sets of constants contained in two different reduced Hamiltonians are two different solutions for the same eigenvalue problem. From equation (II.76), one can say that two different Hamiltonians can be connected by a rotation operator. From equation (II.74):

$$H_2 = \exp([T , *]) H_1 \qquad \text{(IV.1)}$$

which means that H_2 can be obtained from H_1 by applying a rotation involving the transformation operator T. Equation (IV.1) can be written in vector form

$$\mathbf{O}\, \mathbf{h}_2 = \exp([\mathbf{O}, \mathbf{t} , *]) \mathbf{O}\mathbf{h}_1 . \qquad \text{(IV.2)}$$

The vector spaces for the Hamiltonian (without any subindex) and the transformation operator have been discussed in detail in Chapters II and III. Expanding the exponential operator, and truncating the expansion up to first order terms, one obtains

$$O\,h_2 = O\,h_1 - i[\,O,\ t\ ,\ O\,h_1\,]\ . \qquad \text{(IV.3)}$$

The commutator in equation (IV.3) can be written, by the use of the commutation relations between the angular momentum operators, as:

$$\Sigma_i\,\Sigma_j\,\{\,-i\,t_i\,[\,O_{m1,i}\ ,\ O_{m2,j}\,]\,h_{1,j}\,\} = \Sigma_i\,\Sigma_{j=1}\,\Sigma_{k=1}\ t_i\ c_i(k,j)\ O_{m2,k}\ h_{1,j}\ . \qquad \text{(IV.4)}$$

In equation (IV.4), the transformation operators $O_{m1,i}$, the Hamiltonian operators $O_{m2,j}$ and the commutator matrix elements $c_i(k,j)$, do not have any superscript. They can equally be defined as the $O^n_{1,i}$, $O^n_{2,j}$, and $c_i(k,j)$ of the rotor case, as they occur in equations (II.64) and (II.65), or as the $O^{s,n}_{2;i}$, $O^{s,n}_{1;j}$ and $c^s_i(k,j)$ of the spin-rotor case, as they occur in equation (III.63) and (III.64). Rearranging the order of summation in equation (IV.4),

$$\Sigma_i\,\Sigma_j\,\{\,-i\,t_i\,[\,O_{i,i}\ ,\ O_j\,]\,h_{1,j}\,\} = \Sigma^d_{i=1}\{\,\Sigma^d_{k=1}\,O_k\,\Sigma^d_{j=1}\,t_i\,c_i(k,j)\,h_{1,j}\,\}\ . \qquad \text{(IV.5)}$$

In vector and matrix terms this can be written as

$$-\,i[\,O,\ t\ ,\ O\,h_1\,] = \Sigma_i\,O\,t_i\,c_i\,h_1\ . \qquad \text{(IV.6)}$$

Grouping the sum of the commutator matrices into a single

one,

$$C = \Sigma_i t_i c_i , \qquad (IV.7)$$

equation (IV.6) becomes

$$- i[O, t , O h_1] = O C h_1 . \qquad (IV.8)$$

Substituting equation (IV.8) into equation (IV.3), one obtains

$$O h_2 = O h_1 + O C h_1 = O (1 + C) h_1 . \qquad (IV.9)$$

Taking into consideration that equation (IV.9) is the result of truncating the expansion of an exponential operator, the final result should be written as

$$O h_2 = O \exp(C) h_1 \qquad (IV.10)$$

from which one obtains the relation between the two sets of coefficients as

$$h_2 = \exp(C) h_1 . \qquad (IV.11)$$

As discussed above, all the coefficients in equation (IV.11), i.e., the elements of h_1, h_2 and the C matrix, are truncated at a certain order of magnitude for practical

reasons. The exponential operator must be expanded according to the magnitude requirements of the coefficients. For mathematical simplicity, let us assume that the truncation can be done up to first order terms. Then

$$h_2 = h_1 + C\, h_1 \qquad \text{(IV.12)}$$

and, from equation (IV.7):

$$h_2 = h_1 + \Sigma_i\, t_i\, c_i\, h_1 \,. \qquad \text{(IV.13)}$$

Equation (IV.13) is the basis for two methods for switching from one reduced Hamiltonian, with known parameters (h_1), to another with parameters (h_2) to be determined. The rotation method, which is discussed in detail in section C, uses equation (IV.13) directly and therefore involves the determination of the transformation parameters, t_i, as well as solution of the equation to obtain the parameters colected in h_2. The method of invariant combinations is based upon obtaining functions of the h_2 parameters which are equal to the *identical* functions of the h_1 parameters. These functions, which are called invariant combinations, cannot therefore depend upon t_i, i.e., they are invariant under a rotation to the Hamiltonian.

B. INVARIANT COMBINATIONS

As discussed above, the basis for this method of connection between two reductions is

$$f(h_1) = f(h_2) \qquad \text{(IV.14)}$$

i.e., one defines identical functions of the parameters of two Hamiltonians, reduced according to different schemes, which are equal. This section describes the basis for determining these invariant combinations.

The simplest kind of function that can be considered is a linear combination of the Hamiltonian parameters. This kind of function is called a linear invariant combination and can be expressed mathematically as

$$\mathbf{l}\, h_2 = \mathbf{l}\, h_1 \qquad \text{(IV.15)}$$

where $\mathbf{l}$ is a row vector collecting the constants that specify the linear combination. In what follows both $\mathbf{l}h$ and $\mathbf{l}$ will be referred to as invariant combinations because definition of a combination is implicit in $\mathbf{l}$. This usage has the advantage of avoiding the creation of a phrase to distinguish the two forms. The context of the discussion determines which is intended.

From equation (IV.13),

$$1\,h_1 + \Sigma_i\, t_i\, 1\, c_i\, h_1 = 1\, h_1 \,, \qquad \text{(IV.16)}$$

so that

$$\Sigma_i\, t_i\, 1\, c_i = 0 \,. \qquad \text{(IV.17)}$$

Because equation (IV.17) must be valid for any arbitrary values of the t's, the components of 1 satisfy the following equation simultaneously for all c_i

$$1\, c_i = 0 \,. \qquad \text{(IV.18)}$$

The linear invariant combinations are therefore given by the linear combinations of rows of the c_i matrices that simultaneously give a row of zeros.

Because the parameters in the reduced Hamiltonian correspond to terms up to certain order of magnitude, the invariant combinations must also be carried to that order of magnitude. The order of magnitude of an invariant combination is determined by the elements of lowest order of magnitude involved in it. In order to be able to determine the parameters in the Hamiltonian of a certain order of magnitude, it is necessary to have an equal number of invariant combinations of the same order of magnitude, i.e., one must have an equal number of equations and unknowns.

Except in the most trivial case, the number of linear invariant combinations does not provide a complete set of

equations so that one must pass on to consider quadratic invariant combinations. A quadratic invariant combination is a linear combination of second degree products of parameters in the Hamiltonian that is invariant under a rotation. By comparison with equation (IV.4)

$$q(h_2 \times h_2) = q(h_1 \times h_1) \qquad \text{(IV.19)}$$

where the notation $A \times B$ indicates the direct matrix product as defined by Margenau and Murphy[28] and q is a row vector containing the coefficients which define the quadratic invariant combination. As the first step in the determination of q, one substitutes from equation (IV.12) to obtain

$$q\{ (I\, h_1 + C\, h_1) \times (I\, h_1 + C\, h_1) \} = q(h_1 \times h_1) \qquad \text{(IV.20)}$$

where I is the identity matrix. Multiplying this out, one obtains

$$\begin{aligned} q\{ & h_1 \times h_1 + (I\, h_1) \times (C\, h_1) \\ & + (C\, h_1) \times (I\, h_1) + (C\, h_1) \times (C\, h_1) \} \\ & = q(h_1 \times h_1) \,. \end{aligned} \qquad \text{(IV.21)}$$

Since[28]:

$$A \cdot B \times D \cdot E = (A \times D) \cdot (B \times E) \qquad \text{(IV.22)}$$

equation (IV.21) can be resolved to:

$$q\{ I \times I + I \times C + C \times I + C \times C \} (h_1 \times h_1) = q(h_1 \times h_1) \; . \qquad \text{(IV.23)}$$

In equation (IV.23) the last term will be dropped in order to be consistent with the truncation of the equation beyond lowest order terms. From equation (IV.7)

$$I \times C + C \times I = \Sigma_i \, t_i \, (I \times c_i + c_i \times I) = \Sigma_i \, t_i \, c_i^{(2)} \qquad \text{(IV.24)}$$

where

$$I \times I = I \; , \qquad \text{(IV.25)}$$

yields a unit matrix of dimensions twice those of the unit matrices in the product, and

$$c_i^{(2)} = I \times c_i + c_i \times I \; . \qquad \text{(IV.26)}$$

The superscript (2) indicates that the matrices $c_i^{(2)}$ correspond to second degree products of Hamiltonian parameters. Substitution of equation (IV.24) into equation

(IV.23) gives

$$q(I + \Sigma_i t_i c_i^{(2)})(h_1 \times h_1) = q(h_1 \times h_1) , \qquad (IV.27)$$

and finally one obtains the condition which the vector q must satisfy

$$\Sigma_i t_i q c_i^{(2)} = 0 . \qquad (IV.28)$$

Equation (IV.28) is very similar to equation (IV.17), the only difference being the origin of the matrices. The quadratic invariant combinations are given by the linear combinations of the rows of the $c_i^{(2)}$ matrices that simultaneously give rows of zeros.

In some cases it is necessary to go up to higher degree products of the coefficients in the Hamiltonian, until the required number of invariant combinations is obtained. By comparison of equation (IV.19) and equation (IV.28), one can generalize to obtain the equation corresponding to an nth degree invariant combination

$$\Sigma_i t_i n c_i^{(n)} = 0 . \qquad (IV.29)$$

This must be satisfied by the vector of coefficients n corresponding to a linear combination of products of parameters h_i of degree n. The only modification in the procedure for obtaining invariant combinations of different

degrees is the construction of the $c_i^{(n)}$ matrices. From equation (IV.25), one can generalize the manner in which the different matrices are constructed from the single commutator matrices c_i's.

C. CONNECTION BY A ROTATION OF THE HAMILTONIAN

In the previous sections, the application of a rotational transformation to the reduced Hamiltonian in order to obtain a different reduction scheme has been discussed. In equation (IV.13),

$$h_2 = h_1 + \Sigma_i\, t_i\, c_i\, h_1 \,,$$

it is assumed that h_1 is obtained from a fitting procedure and h_2 is the set of parameters in the reduction scheme to which we want to switch. One can divide the set of equations in equation (IV.13) into two sets: one set containing those parameters that are zero in the second reduction scheme, and the other containing the parameters that are to be determined.

The first set satisfy the relation

$$h_1 + \Sigma_i\, t_i\, c_i\, h_1 = 0 \qquad \text{(IV.30)}$$

since the parameters are zero in the second reduction scheme. The number of equations here is equal to the number of parameters in the rotation operator, which means that the

system has an equal number of equations and unknowns (t_i's), and can therefore be solved uniquely to obtain the explicit values for the parameters in the rotation operator.

The remaining set of equations in equation (IV.13) simply relates the parameters in the Hamiltonian reduced according to the second scheme to the parameters in the Hamiltonian reduced according to the original scheme. The new parameters are easily determined since all of the parameters in the rotation operator have been determined by solution of equation (IV.30).

It can be concluded that, by solving the system of equations (IV.13), one can obtain not only a method of transformation between two different schemes of reduction, but also a method for obtaining the parameters involved in the the transformation.

D. COMPARISON OF METHODS FOR CONNECTING DIFFERENT REDUCTIONS

Some details must be emphasized with respect to the two methods described above. Equation (IV.11) is the fundamental relation which is made viable by an expansion of the exponential. In doing the expansion one has to be very careful, in terms of order of magnitude considerations. From the fitting procedure one can only obtain a certain precision in the results, which in turn determines the order of magnitude up to which the treatment may be carried out. Once the order of magnitude is selected, it is the basis for truncation of the Hamiltonian vector and the commutation

matrices. The truncation has also to be consistent when the matrices for higher degree products of Hamiltonian parameters are obtained, as was done in passing from equation (IV.23) to (IV.26).

The invariant combinations and rotation methods described above are, in principle, equally useful in terms of allowing one to switch from one reduction to another. One can choose either of the two methods according to mathematical convenience, i.e., the method which gives the more easily solved set of equations. The rotation method has the advantage of determining the values for the parameters of the rotation involved in the change of reduction scheme. It is shown in Chapter VI that the parameters of the rotation operator give an idea of how much magnitude distortion the Hamiltonian undergoes by the change in reduction scheme. Magnitude distortion means that the order of magnitude classification made in the construction of the model Hamiltonian is not followed by the parameters obtained from the fitting to this model Hamiltonian. If the parameters in the non-reduced Hamiltonian could be known, the second method would also give an indication of the magnitude distortion that is produced in the Hamiltonian by means of the reduction procedure. The magnitude distortion is reflected in the quality of the fit obtained within a scheme of reduction, as will be shown in Chapter VI.

V. INVARIANT COMBINATIONS

A. GENERAL CONSIDERATIONS

The purpose of this Chapter is to analyze the spin-rotor reduction, assuming that the rotor reduction has been done previously. It was shown in Chapter III that this assumption is valid because of the commutation properties of the rotational and spin angular momentum operators. One must choose a specific molecule or group of molecules which satisfy the requirements of the model Hamiltonian which is to be used. The precision of the experimental data gives the order of magnitude to be used for truncating the equations that were discussed in previous Chapters. For the specific case of a molecule with orthorhombic symmetry, and in a doublet state, we have chosen

MOLECULE	NH_2
ORDER OF MAGNITUDE	10
SYMMETRY	ORTHORHOMBIC

Using the information given in equations (II.19), (III.60) and Tables II.2 and III.3, the Hamiltonian truncated at tenth order of magnitude is

$$H = \Sigma^{3}_{l=1}\, h^{0}_{l}\, O^{2}_{2,l} + \Sigma^{3}_{l=1}\, h^{1}_{l}\cdot^{2}\, O^{1}_{1;l} + \Sigma^{6}_{l=1}\, h^{4}_{l}\, O^{4}_{2,l}$$
$$+ \Sigma^{9}_{l=1}\, h^{1}_{l}\cdot^{6}\, O^{1}_{1;l} + \Sigma^{10}_{l=1}\, h^{8}_{l}\, O^{8}_{2,l} + \Sigma^{8}_{l=1}\, h^{1}_{l}\cdot^{10}\, O^{1}_{1;l} \,. \qquad (V.1)$$

The corresponding spin-rotor transformation operator is:

$$T^{1} = \Sigma^{3}_{l=1}\, h^{1}_{l}\cdot^{8}\, O^{2}_{2;l} + \Sigma^{9}_{l=1}\, h^{1}_{l}\cdot^{10}\, O^{1}_{2;l} \,. \qquad (V.2)$$

Taking note of the invariance of the rotor Hamiltonian under the spin-rotor transformation, and expanding equation (III.67) up to the contributions to tenth order of magnitude, one obtains the changes effected by the spin-rotor transformation:

$$H(s\text{-}r)(10)' = H(s\text{-}r)(10) - i\, \Sigma^{3}_{l=1}\, t^{1}_{l}\cdot^{6}\, [\, O^{2}_{2;l}\,,\, H(4)]$$
$$- i\, \Sigma^{9}_{l=1}\, t^{1}_{l}\cdot^{10}\, [\, O^{1}_{2;l}\,,\, H(0)] \,. \qquad (V.3)$$

In equation (V.3), three points should be emphasized:

1) The numbers in parentheses indicate the order of magnitude beyond which the corresponding vector is truncated.

2) The Hamiltonian operator in commutation with the transformation operator is the sum of the rotor and spin-rotor Hamiltonians.

3) For working up to tenth order of magnitude, the expansion of the rotation operator in equation (III.63) can be truncated beyond first order terms and the Hamiltonian

within the two commutators can be truncated at fourth and zeroth order of magnitude.

From equations (III.69) and (IV.8), one can bring equation (V.3) into matrix form:

$$O_i^j\, h'(10)' = O_i^j \{ h'(10) + \Sigma_{j=1}^{3} t_j^{\,8}\, c_j^{\,(10,4)}\, h(4) + \Sigma_{j=1}^{9} t_j^{\,10}\, c_j^{\,(10,0)}\, h(0) \} \qquad (V.4)$$

where the commutator matrices c_j^i are defined in equation (II.64), and the vectors **h** contain the rotor and the spin-rotor parameters. The truncation of the commutator matrices is indicated by a pair of superscripts in parentheses. The matrices arise from commutators between operators associated with the t_j^i and those associated with the parameters in the following **h**. The second superscript therefore indicates truncation of the matrices at the dimensions consistent with the **h** which they multiply. The results of the commutators are the O_i^j associated with the $h'(10)$. The first superscript therefore indicates the corresponding truncation of the commutator matrices.

It is necessary to calculate the 12 commutator matrices that are contained in equation (V.4). The program for this purpose was adapted from the one used in previous work for the rotor case[25]. The names of this and all other programs mentioned in this section are given in Appendix A. As mentioned in Chapters II and III, there are two representations that are commonly used in the literature:

the standard form and the ladder form. The program for calculating the commutator matrices uses the standard form.

The relation between the standard and the ladder form can be represented as,

$$O_d = O_t a \qquad (V.5)$$

with the standard form operators, O_t, being named the t style and the ladder form operators, O_d, the d style. Equation (V.5) can be compared with the basis transformation expressed in equation (II.25). The subindices t and d refer to two different operator bases, and the a matrix is the transformation matrix between these two specific bases.

The a matrix and its inverse, which are calculated with computer programs, can be used for the transformation of the c_i matrices from the t to the d style and vice versa. The relationship between the t style $c_{i,t}$ matrix and the d style $c_{i,d}$ matrix is obtained by recognizing that $O_t c_{i,t} h_t$ is equal to $O_d c_{i,d} h_d$ and, that

$$O_t\, c_{i,t} h_t = O_t\, a\, a^{-1} c_{i,t}\, a\, a^{-1}\, h_t \qquad (V.6)$$

which, with the use of equation (V.5), becomes

$$O_t\, c_{i,t} h_t = O_d\, a^{-1} c_{i,t}\, a\, h_d = O_d\, c_{i,d}\, h_d \,. \qquad (V.7)$$

Thus

$$c_{i,s} = a^{-1} c_{i,r} a \quad . \qquad (V.8)$$

The transformation derived above applies to both the rotor and spin-rotor cases. The $c_{i,r}$, $c_{i,s}$ and a matrices for both cases are available and are stored in the files named in Appendix A.

B. INVARIANT COMBINATIONS FOR THE SPIN-ROTOR HAMILTONIAN

In order to obtain invariant combinations of a certain nth degree, one has to follow three steps:

1) Obtain the transformation matrices $c_j^{(n)}$, by following the logic used to generate the $c_j^{(2)}$ matrices in equation (IV.25). It can be generalized as:

$$c_j^{(n)} = \Sigma_{j=1}^{n} P_j \left(I^{n-1} \times c_i \right) \qquad (V.9)$$

where the $I^{n-1} \times c_i$ means the direct products of the n-1 identity matrices with the c_i matrix, with the sum taken over all the possible permutations, P_j, of the c_i matrix within the multiple direct products.

2) Calculation of the possible combinations of rows of the $c_j^{(n)}$ matrices which simultaneously give a row of zeros. For that purpose, two matrices are needed. One can be called the working matrix, which includes the twelve $c_j^{(n)}$ matrices at the same time, as a series of strips of columns. The second, which can be called the reference matrix, is initially a unit matrix. The number of rows in the working

matrix determines the dimensions of the reference matrix. One performs additions and subtractions among the rows in the working matrix in order to obtain as many zeros as possible across the rows of the matrix. That can be done by a Gauss or Jordan elimination procedure. By carrying these additions and subtractions into the reference matrix as well, one obtains a record of the manipulations done in the working matrix. As a consequence, whenever a certain row of zeros is obtained in the working matrix, the corresponding row of the reference matrix contains an invariant combination.

3) When the invariant combinations of a certain degree have been obtained, they have to be "cleaned". One attempts to express the invariant combinations with the minimum possible number of terms. The cleaning of the invariant combinations can be done by applying a Gauss or Jordan elimination procedure to the rows of the reference matrix which correspond to the invariant combinations.

The above procedure has been carried out for linear up to sextic spin-rotor invariant combinations, using computer programs. The names of all the programs mentioned in this section are contained in Appendix B.

Some of the nth degree invariant combinations so obtained are combinations of products of lower degree invariant combinations, and hence are not unique. For example in the case of the quadratic invariant combinations, one obtains 80 of them, but of these:

24 correspond to the $h_i^0 \cdot$linear type,

9 correspond to the $h_i^1 \cdot$linear type,

42 correspond to the $h_i^2 \cdot$linear type,

1 corresponds to the linear·linear type,

and only 4 correspond to unique quadratic invariant combinations. The notation $h_i \cdot$linear refers to quadratic combinations obtained by multiplying a single Hamiltonian parameter by a linear invariant combination. The notation linear·linear refers to a product of two linear invariant combinations. The final number of invariant combinations obtained for the full determination of the spin-rotor parameters is contained in Table V.1.

TABLE V.1

SPIN-ROTOR INVARIANT COMBINATIONS

	Degree of invariant combinations						
magnitude	1	2	3	4	5	6	Total
2	1	1	1	0	0	0	3
6	3	0	1	2	0	0	6
10	4	3	0	0	1	4	12

The computer programs listed in the Appendix B give the invariant combinations in t style. The transformation from t to d style can be accomplished by use of the a matrix. From equation (IV.15) for the linear case:

$$l_t\, h_t = l_t\, a\, a^{-1}\, h_t \,. \qquad (V.10)$$

From equation (II.25):

$$l_t\, h_t = l_t\, a\, h_d = l_d\, h_d \qquad (V.11)$$

so that

$$l_d = l_t\, a \,. \qquad (V.12)$$

For the quadratic case, from equation (V.8):

$$q_t\, (\, h_t \times h_t\,) = q_t\, (\, a h_d\,) \times (\, a h_d\,) \,. \qquad (V.13)$$

From equation (IV.21):

$$\begin{aligned} q_t\, (\, h_t \times h_t\,) &= q_t\, (\, a \times a\,)\, (\, h_d \times h_d\,) \\ &= q_d\, (\, h_d \times h_d\,) \end{aligned} \qquad (V.14)$$

so that

$$q_d = q_t\, (\, a \times a\,) \,. \qquad (V.15)$$

The same logic is followed to obtain the transformation of invariant combinations from t to d style of the higher degree invariant combinations. The transformations were done with computer programs. Different degrees of cross products

of the a matrix are calculated in order to obtain the transformation matrix from t to d style for different degrees of invariant combinations.

After the invariant combinations are obtained in d style, they also have to be "cleaned". The cleaning procedure is required in order to obtain the invariant combinations with the minimum possible number of elements. The cleaning is done by a Jordan or Gauss elimination procedure within computer programs. The names of the files in which the invariant combinations are contained are given in Appendix B.

Because of the high degree required for obtaining the complete set of invariant combinations, they have a very complex structure which makes it advisable to show that the equations obtained are actually invariant combinations. The verification was done on the computer in a numerical fashion. A set of arbitrary numbers (created by a random number generator) is chosen for the constants (h_1) in the Hamiltonian. A set of arbitrary (random) numbers is also given for the transformation operator constants (t_1) and, using equation (V.4), the parameters (h_2) for the transformed Hamiltonian are calculated. From each set of parameters, values of the invariant combinations are obtained numerically. The numerical values of the invariant combinations calculated from both sets of parameters agree up to the required order of magnitude. The numerical result for the verification is given in Appendix B.

It is evident from Tables III.4 and V.1 that the total number of invariant combinations at tenth order of magnitude obtained (12) is greater than the number actually required (9). There is the possibility that the extra sextic invariant combinations could be linear combinations of lower degree invariant combinations. One has therefore to demonstrate that all of the invariant combinations are linearly independent. The demonstration of linear independence of the invariance relations was done numerically on the computer. One must consider the linear independences corresponding to the invariant combinations of each degree in turn. For the linear case, one has eight invariant combinations, and the following equation can be written to investigate the linear dependence among them:

$$\Sigma_{i=1}^{8} l_{i,j}\, a_i = 0 \qquad \text{(V.16)}$$

where the a_i are unknown constants and

$$l_{i,j} = l_i h_j \; ; \qquad \text{(V.17)}$$

is the numerical result of the ith invariant combination with a specific numerical set of parameters h_j in the Hamiltonian. If the linear invariant combinations are linearly independent, the only solution to equation (V.16) is the trivial solution, in which values of all a_i are zero.

Using an arbitrary set of values for the Hamiltonian parameters, one can compute the values of the invariant combinations numerically. With eight different sets of values for the Hamiltonian parameters, equation (V.16) can be transformed into the following system of equations:

$$\mathbf{L}\,\mathbf{a} = 0 \qquad (V.18)$$

If the determinant of **L** is equal to zero, the invariant combinations are linearly dependent.

For the quadratic case, the linear independence of the four invariant combinations requires that

$$\Sigma_{i=1}^{4}\, q_{i,j}\, a_i = 0 \qquad (V.19)$$

shall have only the solution with all a_i equal to zero. Equation (V.19) is incomplete in the sense that it does not recognize that any bilinear product of linear invariant combinations is itself a quadratic invariant combination

$$q_{i(k,m),j} = l_{k,j} \cdot l_{m,j} \,. \qquad (V.20)$$

Therefore, one has to show that the four quadratic invariant combinations are mutually linearly independent and that they are linearly independent with respect to the bilinear products of the linear invariants.

In principle, equation (V.19) can be extended to,

$$\Sigma_{i=1}^{8} q_{i,j} a_i + \Sigma_{k=1}^{8} \Sigma_{m=1}^{8} l_{k,j}\, l_{m,j}\, a_{i(k,m)} = 0 \qquad (V.21)$$

but, in terms of order of magnitude truncation, only the second and sixth order of magnitude linear invariant combinations need to be considered. Using the information from Table V.1 equation (V.21) is truncated as follows:

$$\Sigma_{i=1}^{8} q_{i,j} a_i + l_{i,j}(2) \cdot l_{i,j}(2) a_s + \Sigma_{i=2}^{8} l_{i,j}(2) \cdot l_{i,j}(6) a_{i-s} = 0 \qquad (V.22)$$

where the numbers in parentheses indicate the order of magnitude of the linear invariant combinations.

Following the procedure established for the linear case, substitution of eight sets of arbritary values of the parameters in the Hamiltonian allows equation (V.22) to be expressed in matrix form as

$$\mathbf{Q}\,\mathbf{a} = 0 \,. \qquad (V.23)$$

A zero value for the determinant of the **Q** matrix verifies that the system is linearly dependent.

For the higher degree invariant combinations, an analogous procedure is employed. One must insure that all possible products of lower degree invariant combinations, which satisfy the order of magnitude restrictions, are

included. The linear independence of all invariant combinations was verified by computer calculations. As a result one can use any one of the four sextic invariant combinations to obtain a complete set of invariant combinations.

The invariant combinations are obtained ultimately in d (or ladder) style, because the reduction schemes are expressed with respect to that style.

Now that the required number of invariant combinations are obtained, one may use them for connection between two different schemes of reduction. The system of equations to be solved is:

$$f_k(\mathbf{h}_1) = f_k(\mathbf{h}_2), \qquad k=1,12 \tag{V.24}$$

with f_k the kth invariant combination. The program used for solving these equations is an adaptation of a program used in previous work[25]. The method used for solving the system of equations is an iterative Newton-Raphson method for many variables.

The results of the A-S reduced spin-rotor Hamiltonian transformation are given in Appendix B. Four different results are shown, corresponding to the use of the four different sextic invariance relations available at tenth order of magnitude. The results clearly show that there is a problem with the invariant combinations method in terms of precision. Because of the high degree that is needed for

obtaining a complete set of invariant combinations, the solution of the equations does not have the required precision. The method was therefore abandoned.

VI. ROTATION METHOD AND ARTIFICIAL SPECTRA

A. ARTIFICIAL SPECTRA

For the fitting of a spectrum, one has to choose a certain scheme of reduction. The choice of a reduction scheme is based on essentially two criteria: the required precision of the final eigenvalues and the rapidity of convergence. It has been shown previously[6] for the rotor Hamiltonian that the A reduction does not work in the case of a molecule that is a near symmetric rotor. Thus it is possible that there may be factors other, than the simple criteria listed, which come into play in the choice of a reduction scheme. Hence it is worthwhile to study the behavior of a reduction scheme in a system for a variety of values of the parameters in the Hamiltonian.

There is an important practical problem in the kind of study described above: NH_2 is the only molecule for which a spectrum with the required precision is available. Because of this, the only alternative is to create artificial spectra, by proposing a series of Hamiltonian parameters which simulate the molecular examples we would like to consider. The matrix elements for the Hamiltonian and the spectra were generated by a computer program adapted from one used in previous work[25]. The name of this and other programs used in this section are listed in Appendix C.

The Hamiltonian parameters for creating artificial spectra should be based upon the information available for a

real molecule. In previous work[17], the zeroth and second order of magnitude constants for NH_2 were obtained, and they are used as a starting point in this work:

TABLE VI.1

DATA FOR THE NH_2 PRINCIPAL CONSTANTS[17]

constant	value (cm^{-1})	operator
A-K	13.12554117	N_z^2
A-N	10.56384184	N^2
a	1.19553384	f^2
(s)A-K	-0.28001133	$N \cdot S$
(s)A-N	-0.24999661	$N_z S_z$
(s)a'	-0.01249793	fF

It should be noted that the numerical orders of magnitude of the constants are within the order of magnitude assumed in the construction of the Hamiltonian (Chapters II and III).

In order to characterize the asymmetry of the molecule, it is useful to introduce the variable K

$$K = \{(A-K)+6a\}/\{(A-K)+2a\} , \qquad (VI.1)$$

which is commonly used in spectroscopy. The range of values of K is from -1 to 1, the lower limit refering to a prolate and the upper limit to an oblate symmetric rotor. A value of K=0 can be interpreted as a completely asymmetric rotor. For

NH_2, the value of K calculated from the data in Table VI.1 is -0.4.

One wants to simulate molecules with different degrees of asymmetry in order to study the influence of the parameter K upon the behavior of a reduction scheme. In order to modify the value of K, using the data from Table VI.1, one need only change the value of the parameter "a". From equation (VI.1) one can calculate the values of "a", corresponding to different values of K's. One should attempt to keep as many similarities as possible between the data used for obtaining artificial spectra and the experimental data available. For that reason the parameter (s)a' is varied along with the parameter "a" for the different K values in order to keep the ratio of these parameters constant. The values of K used, and the corresponding Hamiltonian parameters are given in Table VI.2.

TABLE VI.2

HAMILTONIAN PARAMETERS FOR DIFFERENT ASYMMETRY VALUES

K	a	(s)a'
0	2.1876	-0.0211
-0.25	1.5145	-0.0146
-0.50	0.9347	-0.0090
-0.75	0.4375	-0.0042
-0.90	0.1682	-0.0016
-0.99	0.0164	-0.0002

For the values of the other constants, one must consider the order of magnitude classification of the parameters in the Hamiltonian. In this work, two different cases are considered for assigning values to the higher order of magnitude constants:

1) Without A tendency. For this case all the parameters of a specific order of magnitude have the same value. The orders of magnitude correspond to those specified in Tables 1 and 6.

2) With an A tendency. For this case, the parameters that are eliminated in the A reduction have a higher order of magnitude than the rest of the parameters corresponding to operators of the same degree in the Hamiltonian. A 10^{0} and 10^{-2} A tendency was applied to parameters in the Hamiltonian, i.e., the values given to those parameters which are set to zero in the A reduction were this factor times the value assigned to the other parameter of the same degree.

The artificial spectra contain all possible eigenvalues for N in the range from 0 to 10.

B. METHODOLOGY

The asymmetry, K, and the tendency towards the A reduction are the variables whose influence is studied in this work. Insofar as possible one wishes to distinguish the effects which these variables have on the rotor and spin-rotor parts of the Hamiltonian. Since the basis of the

work is artificial spectra, the separation of these parts can be undertaken by considering three different types of reduction:

1) Reduction in both the rotor and spin-rotor parts.
2) Reduction in the spin-rotor part only.
3) Reduction in the rotor part only.

Finally, the effect of a particular reduction is studied by considering all possible combinations of reduction:

0-0 no reduction, used in generation of the artificial spectra.

A-0 A reduced rotor and non-reduced spin-rotor Hamiltonian.

S-0 S reduced rotor and non-reduced spin-rotor Hamiltonians.

0-A non-reduced rotor and A reduced spin-rotor Hamiltonians.

0-S non-reduced rotor and S reduced spin-rotor Hamiltonians.

A-A A reduced rotor and A reduced spin-rotor Hamiltonians.

A-S A reduced rotor and S reduced spin-rotor Hamiltonians.

S-S S reduced rotor and S reduced spin-rotor

Hamiltonians.

S-A S reduced rotor and A reduced spin-rotor Hamiltonians.

The principal criterion for assessing the quality of a fitting of a reduced Hamiltonian to an artificial spectrum generated within the (0-0) scheme is the standard deviation of the differences between the eigenvalues being fitted and the eigenvalues determined by the fitting procedure. Once again, the use of artificial spectra based upon a non-reduced Hamiltonian provides the possibility of using another criterion: the relative magnitudes of the transformation parameters involved in the rotation to the the Hamiltonian in carrying out the reduction, with respect to the orders of magnitude stated in equations (II.67) and (III.70).

The following sections give the details, results and conclusions based upon this strategy.

C. ROTOR A TENDENCY AND ASYMMETRY

The artificial spectra used in this study were based upon:

1) Inclusion of operators of only second and fourth degree in both the rotor and spin-rotor parts. The parameters corresponding to the fourth degree operators were given values which are a factor of ten smaller than required on magnitude grounds. This is done in order to obtain

reasonable values for the standard deviations.

2) A 10^{0} and a 10^{-2} A tendency was applied to the rotor parameters only.

Since the effect of a rotation of the Hamiltonian is to produce terms of higher magnitude than those included in the generation of the artificial spectra, all parameters up to sixth degree were varied in both rotor and spin-rotor parts of the Hamiltonian. Table VI.3 gives the values of the standard deviations (in MHz) obtained in these fits.

TABLE VI.3

A TENDENCY IN THE ROTOR REDUCTION FOR K=-0.5

	Standard Deviation			
Tendency[1)]	A-A	A-S	S-S	S-A
10^{0}	1.2435	1.1120	0.8736	1.1077
10^{-2}	0.0009	0.0009	0.0004	0.0011

[1)]The A tendency was applied to the rotor parameters only.

The introduction of an A tendency into the rotor Hamiltonian gives a better result for the fitting in all four schemes of reduction. The detailed results, given in Appendix C, show that there is a corresponding lowering of the magnitude distortion.

The artificial spectra used as the basis for Table VI.4 were generated with a 10^{-2} A tendency for all asymmetries. The Table gives the values of the standard deviation (in MHz) obtained in the fittings carried out at various K.

TABLE VI.4

ASYMMETRY IN THE ROTOR AND SPIN-ROTOR REDUCTION

	Standard Deviation			
K	A-A	A-S	S-S	S-A
0	0.0001	0.0001	0.0003	0.0003
-0.25	0.0001	0.0001	0.0001	0.0001
-0.5	0.0009	0.0009	0.0004	0.0011
-0.75	0.0017	0.0008	0.0003	0.0004
-0.9	0.0735	0.0657	0.0013	0.2014
-0.99	*	*	0.0007	1.6393

* For these cases it was not possible to obtain a fit.

The A rotor reduction is very sensitive to changes in the value of K. The sensitivity becomes particularly clear when the value of K is less than -0.8. This is in agreement with the results of Winnewisser[6], who studied the near symmetric rotor molecule DSSD. Even when the spin-rotor part is S reduced, the fitting follows the same pattern. The rotor S reduction is not sensitive to the asymmetry parameter, unless the spin-rotor part is A reduced. It is clear that the spin-rotor A reduction is also dependent on K and this is considered in the next section.

These results exposed a feature of the A reduction which had not been noted before. It appears that a molecule to which the A reduction may be usefully applied must have

an intrinsic A tendency in addition to a value of K reasonably far away from ±1. The fact that the A reduction has been successfully applied to a molecule such as formaldehyde[26], with K=-0.96, indicates that the A tendency may become an overriding factor. A detailed study of this effect is outside the scope of the present work but should be pursued. In this connection it is worth noting that one can detect the A tendency in the rotor Hamiltonian of NH_2 when a fitting in the S reduction is done. The results in Appendix E, in which a fitting to the experimental spectra was carried out, show that the terms f^4, N^2f^4 and f^6, which occur in the S reduced but not in the A reduced Hamiltonian, have coefficients which are at least an order of magnitude smaller than anticipated.

D. SPIN-ROTOR REDUCTION

The artificial spectra generated for the purpose of studying the spin-rotor reduction have the following characteristics:

1) All parameters up to sixth degree in both the rotor and the spin-rotor part are included.

2) The values of the fourth and sixth degree parameters are consistent with the orders of magnitude given in Tables II.2 and III.1, with the exception that a 10^{-2} A tendency is introduced into the rotor and spin-rotor parts in the patterns described in the tables below. In order to isolate, as much as possible, the effects of the spin-rotor

reduction, the fitting was done with a non-reduced rotor and a reduced spin-rotor Hamiltonian.

Tables VI.5 and VI.6 give the standard deviations (in MHz) of the fitting when all the parameters of the rotor and spin-rotor parts are varied in the least squares fitting procedure.

TABLE VI.5

A TENDENCY IN THE SPIN-ROTOR REDUCTION FOR K=-0.5

Tendency		Standard Deviation	
R[1]	S-R[2]	A	S
10^{-2}	10^{-2}	0.0001	0.0019
10^{0}	10^{-2}	0.0010	0.0095
10^{-2}	10^{0}	0.0136	0.0046
10^{0}	10^{0}	0.2191	0.0315

[1] A tendency in the rotor part.

[2] A tendency in the spin-rotor part

TABLE VI.6

A TENDENCY IN THE SPIN-ROTOR REDUCTION FOR K=-0.9

Tendency		Standard Deviation	
R[1]	S-R[2]	A	S
10^{-2}	10^{-2}	0.0067	0.0150
10^{0}	10^{-2}	0.0114	0.0582
10^{-2}	10^{0}	0.8025	0.0415
10^{0}	10^{0}	*	0.4211

[1] A tendency in the rotor part.

[2] A tendency in the spin-rotor part

* For this case it was not possible to obtain a fit.

From Table VI.5 one can say:

1) The introduction of an A tendency into the model Hamiltonian improves the results of the fitting in both schemes of reduction.

2) The A tendency in the rotor part has more influence than in the spin-rotor part when an A reduction is used.

3) The A reduction scheme is more strongly influenced by the A tendency. This is logical since the tendency is towards the A reduction.

From comparison of Tables VI.5 and VI.6, one can conclude that:

1) The general behavior of the schemes of reduction with respect to the A tendency does not depend on the value of K.

2) Both schemes of reduction depend on K, although the A spin-rotor reduction is more sensitive than the S. There are two main reasons why the K parameter, which is a function of the zero order rotor Hamiltonian, affects the spin-rotor reduction: first, as described in the context of equation (III.65), the leading terms for the reduction to the spin-rotor Hamiltonian are commutators between the rotation operator and the zero order rotor Hamiltonian, secondly, the second order spin-rotor Hamiltonian has been made K dependent, as shown in Table VI.1.

Theoretically, it is only possible to use the rotation method for the spin-rotor Hamiltonian when the rotor parameters remain constant in transforming from one reduction to another. In preparation for the application of that method, discussed in section E below, the calculations which led to Tables VI.5 and VI.6 were repeated except that the rotor Hamiltonian parameters were not allowed to vary during the fitting procedure. The results are given in Tables VI.7 and VI.8.

TABLE VI.7

A TENDENCY IN THE SPIN-ROTOR REDUCTION FOR K=-0.5

WITHOUT CHANGES IN THE ROTOR PARAMETERS

Tendency		Standard Deviation	
R[1]	S-R[2]	A	S
10^{-2}	10^{-2}	0.0022	0.0068
10^{0}	10^{-2}	0.0284	0.0158
10^{-2}	10^{0}	0.2144	0.0205
10^{0}	10^{0}	3.5534	0.0505

[1] A tendency in the rotor part.

[2] A tendency in the spin-rotor part

TABLE VI.8

A TENDENCY IN THE SPIN-ROTOR REDUCTION FOR K=-0.9

WITHOUT CHANGES IN THE ROTOR PARAMETERS

Tendency		Standard Deviation	
R[1]	S-R[2]	A	S
10^{-2}	10^{-2}	0.0635	0.1635
10^{0}	10^{-2}	0.2705	0.0898
10^{-2}	10^{0}	0.5961	0.1714
10^{0}	10^{0}	*	0.5768

[1] A tendency in the rotor part.

[2] A tendency in the spin-rotor part

* For this case it was not possible to obtain a fit.

A comparison of standard deviations for the various fittings in Tables VI.5 to VI.8 shows that the spin-rotor

reduction behaves similarly whether or not the rotor parameters participate in the fitting procedure. The main difference is the obtention of a better fitting. This comes from the interplay between the two sets of variables in which adjustment of the rotor parameters accomplishes some of the task which otherwise is done by variation of the spin-rotor set alone. The effect was observable within the correlation matrix of the least squares procedure, where appreciable correlation between the two sets was evident.

The variation of the rotor parameters during the fitting procedure is in contradiction to the requirement that they should remain constant during the spin-rotor reductions considered here. Nevertheless, the empirical evidence arising from the comparison of the two sets of tables is that the pattern of behavior of the spin-rotor reductions is not severely distorted by that variation. This observation suggests a reasonable level of independence between the behaviors of the rotor and spin-rotor reductions. To test this, a set of artificial spectra were produced by a gradual elimination of the spin-rotor parameters. The only reduction done was the rotor reduction, and during the fitting procedure the spin-rotor parameters remained fixed. Table VI.9 gives the standard deviation (in MHz) for all available patterns of A tendency.

TABLE VI.9

A TENDENCY IN THE ROTOR REDUCTION

Spin-rotor parameters[1]	Tendency R[1]	Tendency S-R[2]	Standard Deviation A	Standard Deviation S
all	10^{-2}	10^{-2}	3.2337	0.4612
	10^{0}	10^{-2}	5712.6110	8.7185
	10^{-2}	10^{0}	3.2635	0.4720
2nd. degree	10^{-2}	10^{0}	3.2515	0.4514
	10^{0}	10^{0}	5308.1701	8.7733
none	10^{-2}	10^{0}	3.1323	0.3148
	10^{0}	10^{0}	5167.0053	8.7612

[1] Spin-rotor parameters included for the generation of the spectrum.

[2] A tendency in the rotor part.

[3] A tendency in the spin-rotor part.

One can see that the spin-rotor parameters do not dramatically affect the result of the fitting procedure for a rotor reduction. The dependence of the standard deviation on the A tendency is stronger in the A reduction than in the S reduction. The A tendency has a stronger effect in the rotor reduction. It can be concluded that one must first obtain a good fitting of the spectrum using the rotor parameters, and then improve the result of the fitting by using the spin-rotor part. From Table VI.9 one can see that the spin-rotor parameters are not particularly useful, when the rotor parameters are initially varied. But Tables VI.5

to VI.8 show that the rotor parameters should be used to improve the fitting when the spin-rotor Hamiltonian is being fit. This is in agreement with the mathematical possibility of doing the rotor reduction before the spin-rotor one, but not vice versa.

E. TRANSFORMATION PARAMETERS

Equation (V.4) can be transformed into the following system of equations:

$$h_2^i(10) = h_1^i(10) + \Sigma_{j=1}^{3} t_j^{i,6}\, c^{(10,4)}\, h_1(4) + \Sigma_{j=1}^{9} t_j^{i,10}\, c^{(10,0)}\, h_1(0) \qquad \text{(VI.2)}$$

where the subscripts 1 and 2 differentiate between two sets of Hamiltonian parameters. The name of the computer program used for the solution of equation (VI.2) is given in Appendix D.

The solution can be done for two different purposes:

1) Transformation of a non-reduced spin-rotor Hamiltonian (h_1^i), into a reduced one (h_2^i).

2) Transformation of a spin-rotor Hamiltonian reduced according to a certain scheme (h_1^i) into another reduction scheme (h_2^i).

From the solutions of the equations (VI.2), one obtains the set of parameters in the Hamiltonian to which we want to transform. Also one obtains numerical values for the parameters involved in the transformation operator. In the

non-reduced to reduced transformation, the magnitude of the transformation parameters gives a measure of the magnitude distortion introduced into the Hamiltonian by the reduction procedure. Sometimes the transformation parameters may not follow the order of magnitude classification given in Table III.3. As a result, the orders of magnitude of the parameters in the reduced Hamiltonian are distorted. The eigenvalues obtained by the non-reduced and the reduced Hamiltonian therefore cannot agree to the expected order of magnitude so that, if one produces a spectrum with the non-reduced Hamiltonian, a fitting to the spectrum by the reduction scheme under study will not have the required precision (standard deviation). The presence or absence of the magnitude distortion within the transformation parameters of a reducing rotation therefore serves as a criterion for assessing the selection of a particular reduction.

In principle, the use of equation (VI.2) requires that the rotor parameters be the same in both sets. The style of calculation used in obtaining Tables VI.7 and VI.8 is therefore that which can certainly be used for applying the rotation method to the spin-rotor reduction. The results of the transformation to the A or S spin-rotor reductions for those cases are contained in Tables VI.10 and VI.11. In each case the transformation parameter of largest numerical magnitude is given for the sixth and tenth magnitude transformation.

TABLE VI.10

TRANSFORMATION PARAMETERS[1] FOR K = -0.5

Tendency		A		S	
R[2]	$S-R$[3]	$t^{s,6}$	$t^{s,10}$	$t^{s,6}$	$t^{s,10}$
10^{-2}	10^{-2}	$2\cdot10^{-7}$	$7\cdot10^{-10}$	$2\cdot10^{-8}$	$4\cdot10^{-9}$
	σ	0.0022		0.0068	
10^{0}	10^{-2}	$2\cdot10^{-7}$	$7\cdot10^{-9}$	$2\cdot10^{-6}$	$2\cdot10^{-8}$
	σ	0.0282		0.0158	
10^{-2}	10^{0}	$2\cdot10^{-5}$	$7\cdot10^{-8}$	$6\cdot10^{-6}$	$1\cdot10^{-8}$
	σ	0.2144		0.0205	
10^{0}	10^{0}	$2\cdot10^{-5}$	$7\cdot10^{-7}$	$6\cdot10^{-6}$	$5\cdot10^{-8}$
	σ	3.5534		0.0505	

1) $t^{s,6}$ and $t^{s,10}$ correspond only to the largest absolute value of the whole set specified in equation (VI.2).

2) A tendency in the rotor part.

3) A tendency in the spin-rotor part

TABLE VI.11

TRANSFORMATION PARAMETERS[1] FOR K = -0.9

Tendency		A		S	
$R^{2)}$	$S\text{-}R^{3)}$	$t^{*,6}$	$t^{*,10}$	$t^{*,6}$	$t^{*,10}$
10^{-2}	10^{-2}	$7\cdot10^{-8}$	$2\cdot10^{-7}$	$9\cdot10^{-6}$	$1\cdot10^{-7}$
	σ	0.0635		0.1635	
10^{0}	10^{-2}	$1\cdot10^{-5}$	$1\cdot10^{-6}$	$4\cdot10^{-6}$	$1\cdot10^{-6}$
	σ	0.2705		0.0898	
10^{-2}	10^{0}	$7\cdot10^{-4}$	$2\cdot10^{-5}$	$3\cdot10^{-5}$	$4\cdot10^{-7}$
	σ	1.5961		0.1714	
10^{0}	10^{0}	$1\cdot10^{-4}$	$1\cdot10^{-4}$	$1\cdot10^{-5}$	$3\cdot10^{-6}$
	σ	28.2679		0.5768	

1) $t^{*,6}$ and $t^{*,10}$ correspond only to the largest absolute value of the whole set specified in equation (VI.2).

2) A tendency in the rotor part.

3) A tendency in the spin-rotor part

The detailed values for the transformation parameters are given in Appendix D. The standard deviations (σ in MHz) have been carried forward from Tables VI.7 and VI.8 to aid comparison. There is no doubt that the quality of a fitting reflects the magnitude of the transformation coefficients which also influences the magnitude distortion in the Hamiltonian parameters.

As noted above, the rotation method can also be used for relating two different schemes of reduction. Presume that a good fitting is obtained within a certain reduction. One calculates the required parameters for the transformation to a second reduction. The values of the transformation parameters indicate the quality of the fitting that can be obtained by the second reduction in comparison with the first one. If the transformation parameters are not magnitude distorted, the Hamiltonian parameters h_2 obtained from equation (VI.2) will be very close to those that would be obtained by a fitting procedure. The result serves as an excellent starting point for a fitting. Conversely, when the transformation parameters exhibit magnitude distortion, one has received a warning that the fitting with the second reduction will give rise to problems, including a poor quality of fitting.

In Appendix D the results of the rotation method in the A to S spin-rotor Hamiltonian transformation are given, for the cases in Tables VI.7 and VI.8. By comparison of the results in Appendices C and D, one can see the evidence for

the conclusions given above.

The reduced Hamiltonian obtained by a fitting procedure does not agree completely with the one obtained from equation (VI.2). The reason for the difference is the different information used by the two methods. The least squares fitting uses, for each constant that is being determined, the following information:

1) The matrix elements of the corresponding operator,
2) Derivatives of the term values with respect to the Hamiltonian parameters,
3) The set of experimental term values or transition frequencies.

The rotation method uses, for each constant that is being determined, the following information:

1) The commutator matrices between the Hamiltonian operators and the transformation operators,
2) The value of the constant in the initial reduction,
3) The transformation operator constants.

The magnitudes of the differences in the parameters obtained by the two methods have been shown to be related to the magnitude of the transformation parameters. Therefore, if the transformation parameters are within the order of magnitude classification contained in Table III.3, they will be a good starting point for a fitting.

In conclusion, one can say that the rotation method is highly useful for comparison of different reduced Hamiltonians.

F. EXPERIMENTAL NH2 SPECTRUM

It has been pointed out above that NH_2 is the only molecule with an available experimental spectrum[9-17] of the precision considered in this thesis. The experimental results used in this work are: MODR (microwave-optical double resonance) frequencies[9-13], LMR (laser-magnetic resonance) frequencies[14], combination differences derived from the optical electronic absorption spectrum[15-16] and some term values and combination differences derived from the optical electronic emission spectrum[17].

The artificial spectra generated, for the studies discussed above, contained term values restricted to a maximum of N=10. In order to be able to compare the experimental and artificial spectra results, the first fittings were done with NH_2 spectral data also truncated beyond N=10. The results for the A-A and S-S fittings to the truncated NH_2 spectrum are given in Appendix E. The main points to consider from the results and experience of the two fittings are:

1) There is no appreciable difference in the standard deviation obtained by both schemes of reduction.
2) One has to obtain a good fitting with the rotor parameters before introducing variation of the spin-rotor part.
3) In the results of the S-S fitting, the values of the parameters eliminated in the the A-A reduction have

a higher order of magnitude than expected which means that the molecule has an intrinsic A tendency.

One can conclude that the results obtained by the study of artificial spectra can be applied to experimental situations. One has to be careful to use as much experimental information as possible for the production of artificial spectra because the information that one can obtain from this kind of study is always comparative.

Finally, the A-A and S-S fittings to the complete NH_2 spectrum are reported in Appendix E. The fittings were done by using, as a starting point, the Hamiltonians obtained from the fittings to the truncated spectrum. It is evident that the introduction of data corresponding to higher values of N gives rise to corrections of high order of magnitude to the Hamiltonian constants.

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APPENDIX A

Commutator matrices for the Rotor Hamiltonian:
In t style, file: CM.T; in d style, file: CM.D.

Commutator matrices for the Spin-Rotor Hamiltonian
In t style, file: S.CM.T; in d style, file: S.CM.D

Transformation matrices between d and t style for the Rotor Hamiltonian:
a,file: ALP; a^{-1}, file: ALPI

Transformation matrices between d and t style for the Spin-Rotor Hamiltonian:
a,file: S.ALP; a^{-1}, file: S.ALPI

APPENDIX B

Programs for the generation of the invariant combinations:

linear	nl10.1	quartic	nqq10.1
quadratic	nq10.1	quintic	ncc10.1
cubic	nc10.1	sextic	ns10.1

Programs for the t to d transformation of the invariant combinations, by using the a matrices:

linear	n.dtl	quartic	n.dtqq
quadratic	n.dtq	quintic	n.dtcc
cubic	n.tdc	sextic	n.dts

Programs for the cleaning of the invariant combinations in d style:

linear	n.dtl1
quadratic	n.dtq1
cubic	n.tdc1

Names of the files in which the invariant combinations are contained:

degree	in t style	in d style
linear	MLT10	MLD10
quadratic	MQT10	MQD10
cubic	MCT10	MCD10
quartic	MQQT10	MQQD10
quintic	MCCT10	MCCD10
sextic	MST10	MSD10

Program for the verification of rotational invariance of the invariant combinations in d style: PIR.10.

Results for the verification of rotational invariance of the invariant combinations in d style:

VALUES FOR SET 1	VALUES FOR SET 2	DIFFERENCE
0.1999620591E-01	0.1999620591E-01	0.3469446952E-17
-0.2481660901E-05	-0.2481660901E-05	0.0
0.1140593579E-05	0.1140593579E-05	0.8470329473E-21
0.2095188380E-05	0.2095188380E-05	0.1482307658E-20
0.3972212539E-09	0.3972212539E-09	0.5169878828E-25
-0.6663924218E-09	-0.6663924218E-09	0.5169878828E-25

-0.5367514625E-08	-0.5367514625E-08	0.6617444900E-23
0.3622080983E-09	0.3622080983E-09	0.2067951531E-24
0.4098337104E-01	0.4098337148E-01	0.4400078435E-09
0.9114233073E-09	0.9117633650E-09	0.3400577151E-12
-0.2084489157E-08	-0.2086346247E-08	0.1857089807E-11
0.2007195796E-08	0.2008722830E-08	0.1527034050E-11
-0.6930401794E-01	-0.6930401882E-01	0.8783458405E-09
0.3474662858E-05	0.3475748370E-05	0.1085512121E-08
0.4694246904E-05	0.4694241258E-05	0.5646172083E-11
0.4528810732E-05	0.4528093873E-05	0.7168589292E-09
-0.5485762443E-07	-0.4567843811E-07	0.9179186321E-08
-0.9067044557E-08	-0.9065202734E-08	0.1841822339E-11
-0.1143898210E-07	-0.1144301607E-07	0.4033963938E-11
0.3854100851E-07	0.3854944340E-07	0.8434893146E-11
-0.2566561518E-07	-0.2569570569E-07	0.3009051276E-10

Programs for the verification of the linear independence of the invariant combinations:

linear	LIL10	quartic	LIQQ10
quadratic	LIQ10	quintic	LICC10
cubic	LIC10	sextic	LIS10

Solution of the invariant combinations for the transformation from the A reduced to the S reduced parameters: Program : S.ES10

Results of the A-S transformation, by using the invariant combinations:

	EQUATION 1	
A1	0.1100000000E+01	
A2	0.1200000000E+01	
A3	0.1300000000E+01	
A4	0.1110000000E-03	
A5	0.1220000000E-03	
A6	0.1330000000E-03	
A7	0.1440000000E-03	
A8	0.1550000000E-03	
A9	0.1660000000E-03	
1	0.1110000000E-01	0.1114497346E-01
2	0.1220000000E-01	0.1206906248E-01
3	0.1330000000E-01	0.1326983663E-01
4	0.1110000000E-05	0.5088166302E-05
5	0.1220000000E-05	-0.7261824857E-05
6	----------	----------
7	0.1440000000E-05	-0.5526448966E-05
8	0.1550000000E-05	0.2151440444E-04
9	----------	----------
10	0.1770000000E-05	0.1767696000E-05
11	----------	0.1844317668E-05
12	0.1990000000E-05	----------
13	0.1110000000E-09	0.1027848845E-08
14	0.1220000000E-09	-0.1036678170E-08
15	----------	----------
16	0.1440000000E-09	-0.8885146023E-09
17	0.1550000000E-09	-0.1177818665E-08
18	----------	----------
19	0.1770000000E-09	0.4650000000E-09
20	----------	----------
21	----------	-0.9621221137E-10
22	0.2000000000E-09	0.2791411243E-09
23	0.2110000000E-09	0.5230518303E-08
24	----------	----------
25	----------	----------
26	----------	0.6077281346E-09
27	----------	----------
28	0.2660000000E-09	----------
29	----------	----------

30	0.2880000000E-09	----------

EQUATION 2

A1	0.1100000000E+01	
A2	0.1200000000E+01	
A3	0.1300000000E+01	
A4	0.1110000000E-03	
A5	0.1220000000E-03	
A6	0.1330000000E-03	
A7	0.1440000000E-03	
A8	0.1550000000E-03	
A9	0.1660000000E-03	
1	0.1110000000E-01	0.1114422046E-01
2	0.1220000000E-01	0.1207132149E-01
3	0.1330000000E-01	0.1327021314E-01
4	0.1110000000E-05	0.5088166302E-05
5	0.1220000000E-05	-0.7261848332E-05
6	----------	----------
7	0.1440000000E-05	-0.5526403748E-05
8	0.1550000000E-05	0.2151440616E-04
9	----------	----------
10	0.1770000000E-05	0.1767696000E-05
11	----------	0.1844318421E-05
12	0.1990000000E-05	----------
13	0.1110000000E-09	0.1027848853E-08
14	0.1220000000E-09	-0.1014138372E-08
15	----------	----------
16	0.1440000000E-09	-0.9335959582E-09
17	0.1550000000E-09	-0.1177811704E-08
18	----------	----------
19	0.1770000000E-09	0.4650000000E-09
20	----------	----------
21	----------	-0.9621221317E-10
22	0.2000000000E-09	0.2791329569E-09
23	0.2110000000E-09	0.5230514301E-08
24	----------	----------
25	----------	----------
26	----------	0.6077275602E-09
27	----------	----------
28	0.2660000000E-09	----------
29	----------	----------
30	0.2880000000E-09	----------

EQUATION 3

A1	0.1100000000E+01	
A2	0.1200000000E+01	
A3	0.1300000000E+01	
A4	0.1110000000E-03	
A5	0.1220000000E-03	
A6	0.1330000000E-03	
A7	0.1440000000E-03	
A8	0.1550000000E-03	
A9	0.1660000000E-03	
1	0.1110000000E-01	0.1114996699E-01

2	0.1220000000E-01	0.1205408188E-01
3	0.1330000000E-01	0.1326733987E-01
4	0.1110000000E-05	0.5088166302E-05
5	0.1220000000E-05	-0.7261669204E-05
6	----------	----------
7	0.1440000000E-05	-0.5526748765E-05
8	0.1550000000E-05	0.2151439297E-04
9	----------	----------
10	0.1770000000E-05	0.1767696000E-05
11	----------	0.1844312675E-05
12	0.1990000000E-05	0.0----------
13	0.1110000000E-09	0.1027848798E-08
14	0.1220000000E-09	-0.1186119749E-08
15	----------	----------
16	0.1440000000E-09	-0.5896197802E-09
17	0.1550000000E-09	-0.1177864821E-08
18	----------	----------
19	0.1770000000E-09	0.4650000000E-09
20	----------	----------
21	----------	-0.9621219950E-10
22	0.2000000000E-09	0.2791952676E-09
23	0.2110000000E-09	0.5230544855E-08
24	----------	----------
25	----------	----------
26	----------	0.6077319455E-09
27	----------	----------
28	0.2660000000E-09	----------
29	----------	----------
30	0.2880000000E-09	----------

EQUATION 4

A1	0.1100000000E+01	
A2	0.1200000000E+01	
A3	0.1300000000E+01	
A4	0.1110000000E-03	
A5	0.1220000000E-03	
A6	0.1330000000E-03	
A7	0.1440000000E-03	
A8	0.1550000000E-03	
A9	0.1660000000E-03	
1	0.1110000000E-01	0.1114300725E-01
2	0.1220000000E-01	0.1207496111E-01
3	0.1330000000E-01	0.1327081974E-01
4	0.1110000000E-05	0.5088166302E-05
5	0.1220000000E-05	-0.7261886157E-05
6	----------	----------
7	0.1440000000E-05	-0.5526330891E-05
8	0.1550000000E-05	0.2151440895E-04
9	----------	----------
10	0.1770000000E-05	0.1767696000E-05
11	----------	0.1844319634E-05
12	0.1990000000E-05	----------
13	0.1110000000E-09	0.1027848864E-08
14	0.1220000000E-09	-0.9778207336E-09

15	----------	----------
16	0.1440000000E-09	-0.1006234067E-08
17	0.1550000000E-09	-0.1177800490E-08
18	----------	----------
19	0.1770000000E-09	0.4650000000E-09
20	----------	----------
21	----------	-0.9621221607E-10
22	0.2000000000E-09	0.2791197965E-09
23	0.2110000000E-09	0.5230507853E-08
24	----------	----------
25	----------	----------
26	----------	0.6077266348E-09
27	----------	----------
28	0.2660000000E-09	----------
29	----------	----------
30	0.2880000000E-09	----------

APPENDIX C

Program used for the generation of the spectra: TMV.

Program used for the fitting to the spectra: PDN.

In the fittings that are shown below:

Number = number of term values used for the spectra fitting.
Standard Deviation = overall standard deviation of observed - calculated eigenvalues.
Source = Origin of data; CALC indicates artificial spectra.

With respect to each parameter:

Standard deviation = value of the standard deviation for each constant obtained during the fitting.
cm^{-1} = value for the constant obtained during the fitting in cm^{-1}.
Ratio = standard deviation for the constant / value of the constant.

The constants correspond to the following operators:

Rotor Hamiltonian		Spin-rotor Hamiltonian	
constant	operator	constant	operator
A-K	N_z^2	(S)A-K	N_zS_z
A-N	N^2	(S)A-N	$N\cdot S$
a	f^2	(S)a'	fF
D-KK	N_z^4	(S)D-KK	$N_z^3S_z$
D-KN	$N^2N_z^2$	(S)D-KN	$N_z^2(N\cdot S)$
		(S)D-NK	$N^2N_zS_z$
D-NN	N^4	(S)D-NN	$N^2(N\cdot S)$
d-K	$N_z^2f^2$	(S)d-K	$f^2N_zS_z$
		(s)d-K'	N_z^2fF
d-N	N^2f^2	(S)d-N'	$f^2(N\cdot S)$
		(S)d-N	N^2fF
d	f^4	(s)d	f^3F
H-KKK	N_z^6	(S)H-KKK	$N_z^5S_z$
H-KKN	$N_z^4N_z$	(S)H-KKN	$N_z^4(N\cdot S)$
		(S)H-KNK	$N_z^2N^2N_zS_z$
H-KNN	$N^4N_z^2$	(S)KNN	$N^2N_z^2(N\cdot S)$
		(S)NNK	$N^4N_zS_z$
H-NNN	N^6	(S)H-NNN	$N^4(N\cdot S)$
h-KK	$N_z^4f^2$	(S)h-KK	$N_z^2f^2N_zS_z$
		(S)h-KK'	N_z^4fF
h-KN	$N^2N_z^2f^2$	(S)h-KN	$N_z^2f^2(N\cdot S)$
		(S)h-NK	$N^2f^2N^zS_z$
		(S)h-NK'	$N^2N_z^2fF$
h-NN	N^4f^2	(S)h-NN	$N^2f^2(N\cdot S)$
		(s)h-NN'	N^4fF
h-K	$N_z^2f^4$	(S)h-K	$f^4N_zS_z$

		(S)h-K'	N^2f^3F
h-N	N^2f^4	(S)h-N	$f^4(N\cdot S)$
		(S)h-N'	N^2f^3F
h'	f^6	(S)h'	f^5F

A-A FITTING FOR A MOLECULE WITH K = -0.5
AND WITHOUT A TENDENCY

Source	Number	Std. Dev.	Scaled
CALC	241	0.0000 Cm-1	0.0000
All	241	1.2435 MHz	0.0000
Ratio	Cm-1	Std. Dev.	
0.0000	1.31269399E+01	2.15990644E-06	A-K
0.0000	1.05634430E+01	5.69653615E-07	A-N
0.0000	9.34719983E-01	3.64695173E-07	a
0.0001	1.10055039E-03	1.42228759E-07	D-KK
0.0001	-1.10033276E-03	1.33822378E-07	D-KN
0.0000	2.99975643E-04	6.50276258E-09	D-NN
0.0001	2.92259694E-03	1.71700671E-07	d-K
0.0000	1.00388002E-04	4.30531295E-09	d-N
0.0284	1.65011276E-07	4.69253310E-09	H-KKK
0.0208	-2.57635423E-07	5.34676447E-09	H-KKN
0.0220	8.44831916E-08	1.85536276E-09	H-KNN
0.0025	-3.79264222E-06	9.50348032E-09	h-KK
0.0042	-3.87129052E-07	1.62007924E-09	h-KN
0.0029	-6.30378214E-09	1.83166960E-11	L-KKKK
0.0044	9.74284730E-09	4.24561554E-11	L-KKKN
0.0093	-3.46686896E-09	3.23586819E-11	L-KKNN
0.0360	1.82764190E-09	6.57098553E-11	l-KKN
0.0000	-2.79053395E-01	1.32255980E-05	(S)A-K
0.0002	-2.35810461E-02	5.35954978E-06	(S)A-N
0.0004	-9.00222602E-03	3.91985592E-06	(S)a'
0.0835	8.34538186E-06	6.96583201E-07	(S)D-KK
0.0697	-8.17024646E-06	5.69196827E-07	(S)D-NK
0.0247	3.08572385E-06	7.62183056E-08	(S)D-NN
0.3616	-4.72629808E-06	1.70924848E-06	(S)d-K
0.0264	1.84188740E-06	4.86426099E-08	(S)d-N
0.1939	-2.56277653E-07	4.96964336E-08	(S)H-KKK
0.1866	3.83889310E-07	7.16434458E-08	(S)H-KNK
0.1756	-1.24325477E-07	2.18361447E-08	(S)H-NNK
0.1957	-4.36138800E-07	8.53582820E-08	(S)h-KK
0.4680	3.11787922E-08	1.45908134E-08	(S)h-KN

A-S FITTING FOR A MOLECULE WITH K = -0.5
AND WITHOUT A TENDENCY

Source	Number	Std. Dev.	Scaled
CALC	241	0.0000 Cm-1	0.0000
All	241	1.1120 MHz	0.0000
Ratio	Cm-1	Std. Dev.	
0.0000	1.31269401E+01	1.93112409E-06	A-K
0.0000	1.05634430E+01	5.08667740E-07	A-N

0.0000	9.34720027E-01	3.26096791E-07	a
0.0001	1.10054932E-03	1.27128886E-07	D-KK
0.0001	-1.10033920E-03	1.19584383E-07	D-KN
0.0000	2.99976664E-04	5.80719785E-09	D-NN
0.0001	2.92247695E-03	1.54090006E-07	d-K
0.0000	1.00389017E-04	3.85163013E-09	d-N
0.0249	1.70397018E-07	4.24671400E-09	H-KKK
0.0184	-2.65218269E-07	4.86733219E-09	H-KKN
0.0194	8.66493683E-08	1.67765095E-09	H-KNN
0.0023	-3.78076453E-06	8.62291966E-09	h-KK
0.0038	-3.86273688E-07	1.45101055E-09	h-KN
0.0026	-6.30649468E-09	1.63829705E-11	L-KKKK
0.0039	9.74471772E-09	3.79624865E-11	L-KKKN
0.0083	-3.46573402E-09	2.89309322E-11	L-KKNN
0.0329	1.79104855E-09	5.89476208E-11	l-KKN
0.0000	-2.79062421E-01	1.07704232E-05	(S)A-K
0.0001	-2.35745972E-02	3.09725785E-06	(S)A-N
0.0003	-9.01205068E-03	3.01381896E-06	(S)a'
0.0300	1.20957962E-05	3.62681427E-07	(S)D-KK
0.0266	-1.15102123E-05	3.06055639E-07	(S)D-NK
0.0117	3.34007750E-06	3.91965823E-08	(S)D-NN
0.0181	1.99004983E-06	3.59781922E-08	(S)d-N
0.1073	-1.55425929E-07	1.66697632E-08	(S)d'
0.1699	3.35274439E-08	5.69651079E-09	(S)H-KKK
0.0822	-2.04108843E-06	1.67857049E-07	(S)H-KKN
0.0824	2.00832171E-06	1.65394515E-07	(S)H-KNK

S FITTING FOR A MOLECULE WITH K = -0.5
AND WITHOUT A TENDENCY

Source	Number	Std. Dev.	Scaled
CALC	241	0.0000 Cm-	0.0000
All	241	0.8736 MHz	0.0000
Ratio	Cm-1	Std. Dev.	
0.0000	1.31254820E+01	7.63515023E-07	A-K
0.0000	1.05638609E+01	2.27533738E-07	A-N
0.0000	9.37642469E-01	1.91359011E-07	a
0.0004	6.41222256E-05	2.82289272E-08	D-KK
0.0002	1.43251877E-04	2.49347536E-08	D-KN
0.0000	9.27085385E-05	2.46917668E-09	D-NN
0.0000	9.98900820E-05	2.06988789E-09	d-N
0.0000	1.03568804E-04	4.24981061E-09	d
0.0818	-3.41915524E-09	2.79813119E-10	H-KKN
0.0759	3.00068898E-09	2.27700364E-10	H-KNN
0.0792	5.34039604E-10	4.22735977E-11	h-N
0.0113	7.68467011E-10	8.65519887E-12	h
0.0000	-2.79092155E-01	1.04078820E-05	(S)A-K
0.0002	-2.35622957E-02	4.55611074E-06	(S)A-N
0.0003	-9.01215952E-03	2.39431832E-06	(S)a'
0.0892	3.56023585E-06	3.17453140E-07	(S)D-NK
0.2188	6.27079727E-07	1.37229208E-07	(S)D-NN
0.0667	1.82127924E-06	1.21478975E-07	(S)d-N
0.0610	1.12087250E-06	6.83342335E-08	(S)d'
0.7191	6.57899974E-08	4.73111825E-08	(S)H-KNK

0.7027	-8.10528000E-08	5.69567646E-08	(S)H-NNK
0.6696	1.43279900E-08	9.59428216E-09	(S)H-NNN
0.7013	1.87928566E-07	1.31788696E-07	(S)h-KN
0.7177	-6.82752163E-09	4.89993470E-09	(S)h-N

S-A FITTING FOR A MOLECULE WITH K = -0.5
AND WITHOUT A TENDENCY

CALC	241	0.0000 Cm-1	0.0000
All	241	1.1076 MHz	0.0000
Ratio	Cm-1	Std. Dev.	
0.0000	1.31254816E+01	9.68100970E-07	A-K
0.0000	1.05638611E+01	2.88667581E-07	A-N
0.0000	9.37642607E-01	2.42598672E-07	a
0.0006	6.41247899E-05	3.58361747E-08	D-KK
0.0002	1.43255908E-04	3.16150417E-08	D-KN
0.0000	9.27070813E-05	3.13270486E-09	D-NN
0.0000	9.98881219E-05	2.62397510E-09	d-N
0.0001	1.03568526E-04	5.37669845E-09	d
0.1047	-3.39323036E-09	3.55301246E-10	H-KKN
0.0977	2.95773956E-09	2.89005436E-10	H-KNN
0.1044	5.11992121E-10	5.34420231E-11	h-N
0.0146	7.50243036E-10	1.09611930E-11	h
0.0000	-2.79077605E-01	1.07631795E-05	(S)A-K
0.0002	-2.35675102E-02	3.72027480E-06	(S)A-N
0.0004	-9.04070106E-03	3.17526998E-06	(S)a'
0.0615	9.36865261E-06	5.76095808E-07	(S)D-KK
0.0552	-8.72734952E-06	4.81649490E-07	(S)D-NK
0.0202	2.88651571E-06	5.81961146E-08	(S)D-NN
0.0261	3.50145430E-05	9.15150520E-07	(S)d-K
0.0242	1.82246711E-06	4.41773886E-08	(S)d-N
0.1252	-3.44543650E-07	4.31237461E-08	(S)H-KKK
0.1251	4.90848591E-07	6.14112222E-08	(S)H-KNK
0.1266	-1.46927103E-07	1.86010454E-08	(S)H-NNK
0.1291	-6.72364790E-07	8.68269398E-08	(S)h-KK

A-A FITTING FOR A MOLECULE WITH K = -0.5,
A TENDENCY = 10^{-2} IN THE ROTOR PART ONLY

Source	Number	Std. Dev.	Scaled
CALC	241	0.0000 Cm-1	0.0000
All	241	0.0009 MHz	0.0000
Ratio	Cm-1	Std. Dev.	
0.0000	1.31255546E+01	1.00958102E-09	A-K
0.0000	1.05638378E+01	3.57360189E-10	A-N
0.0000	9.37510628E-01	2.32365195E-10	a
0.0000	1.10006705E-04	3.75799474E-11	D-KK
0.0000	8.79963600E-05	3.18072988E-11	D-KN
0.0000	1.02000031E-04	4.12424529E-12	D-NN
0.0000	1.27984695E-04	9.05435581E-11	d-K
0.0000	1.00002722E-04	2.82131306E-12	d-N
0.0012	1.96936011E-09	2.33286518E-12	H-KKK
0.0012	-2.81103724E-09	3.35189578E-12	H-KKN
0.0012	8.42988043E-10	1.04597335E-12	H-KNN

0.0046	1.00485160E-09	4.61839953E-12	h-KK
0.0003	-2.72118508E-09	8.23396987E-13	h-KN
0.0000	-2.79069159E-01	9.70377428E-09	(S)A-K
0.0000	-2.35710641E-02	4.02402850E-09	(S)A-N
0.0000	-9.06236820E-03	2.96213418E-09	(S)a'
0.0001	1.22286923E-05	1.18116431E-09	(S)D-KK
0.0008	-9.76990415E-05	8.03132893E-08	(S)D-KN
0.0009	8.64736813E-05	7.92853517E-08	(S)D-NK
0.0000	3.00008831E-06	5.53554937E-11	(S)D-NN
0.0000	2.96137880E-05	1.39273089E-09	(S)d-K
0.0000	2.00272280E-06	4.26467333E-11	(S)d-N
0.0226	1.98914689E-09	4.49351610E-11	(s)H-KKK
0.0204	-3.20208029E-09	6.53652541E-11	(S)H-KNK
0.0563	1.14391434E-08	6.44493131E-10	(S)H-KNN
0.0621	-1.02252591E-08	6.35394803E-10	(S)H-NNK
0.1390	6.39559526E-10	8.89093165E-11	(S)h-KK
0.0046	-2.69368243E-09	1.25178185E-11	(S)h-KN

A-S FITTING FOR A MOLECULE WITH K = -0.5,
A TENDENCY = 10^{-2} IN THE ROTOR PART ONLY

Source	Number	Std. Dev.	Scaled
CALC	241	0.0000 Cm-1	0.0000
All	241	0.0009 MHz	0.0000
Ratio	Cm-1	Std. Dev.	
0.0000	1.31255552E+01	9.61957214E-10	A-K
0.0000	1.05638378E+01	3.60288090E-10	A-N
0.0000	9.37510667E-01	2.26567204E-10	a
0.0000	1.10006826E-04	3.89171620E-11	D-KK
0.0000	8.79960389E-05	3.28533478E-11	D-KN
0.0000	1.02000021E-04	4.13360410E-12	D-NN
0.0000	1.27984623E-04	8.95899074E-11	d-K
0.0000	1.00002714E-04	2.85793819E-12	d-N
0.0012	1.97012319E-09	2.37858390E-12	H-KKK
0.0012	-2.81215092E-09	3.41612393E-12	H-KKN
0.0013	8.43378472E-10	1.06501289E-12	H-KNN
0.0047	1.00642324E-09	4.71285146E-12	h-KK
0.0003	-2.72127248E-09	8.26292801E-13	h-KN
0.0000	-2.79083944E-01	1.20667394E-08	(S)A-K
0.0000	-2.35668408E-02	5.04393779E-09	(S)A-N
0.0000	-9.03267484E-03	4.82365873E-09	(S)a'
0.0021	2.81702990E-07	5.79270036E-10	(S)D-KK
0.0051	1.10355755E-05	5.61718244E-08	(S)D-KN
0.0069	-8.20322388E-06	5.70040688E-08	(S)D-NK
0.0005	8.82957946E-07	4.17690437E-10	(S)D-NN
0.0008	2.00626195E-06	1.62451510E-09	(S)d-N
0.0001	1.05903924E-06	9.10971265E-11	(S)d'
0.1449	-1.26918467E-10	1.83883636E-11	(S)H-KKK
0.2637	-2.12803828E-09	5.61174427E-10	(S)H-KNK
0.2562	2.72662277E-09	6.98567663E-10	(S)H-NNK
0.2539	-4.68356896E-10	1.18924053E-10	(S)H-NNN
0.2579	-6.31460798E-09	1.62852544E-09	(S)h-KN
0.4117	2.51504783E-12	1.03550939E-12	(S)h-NN
0.2537	2.34010993E-10	5.93747638E-11	(S)h-N

0.0807	-2.32568095E-12	1.87669622E-13	(S)h'

S-S FITTING FOR A MOLECULE WITH K = -0.5,
A TENDENCY = 10^{-2} IN THE ROTOR PART ONLY

Source	Number	Std. Dev.	Scaled
CALC	241	0.0000 Cm-1	0.0000
All	241	0.0004 MHz	0.0000
Ratio	Cm-1	Std. Dev.	
0.0000	1.31254913E+01	4.60287733E-10	A-K
0.0000	1.05638561E+01	1.94434934E-10	A-N
0.0000	9.37638654E-01	2.01512177E-10	a
0.0000	6.42736054E-05	1.43299935E-11	D-KK
0.0000	1.42862367E-04	1.74171680E-11	D-KN
0.0000	9.28574914E-05	5.30218681E-12	D-NN
0.0000	1.00000125E-04	5.33580045E-12	d-N
0.0000	4.57192855E-06	1.86575163E-12	d
0.0000	-2.00490647E-09	9.98360598E-14	H-KKK
0.0003	-6.33039649E-10	1.98644284E-13	H-KKN
0.0000	3.33615212E-09	1.50888520E-13	H-KNN
0.0000	-6.99029216E-10	3.48055417E-14	H-NNN
0.0022	-1.53566976E-11	3.37486537E-14	h-NN
0.0001	3.49688231E-10	1.87292834E-14	h-N
0.0003	1.53625045E-11	3.85891710E-15	h
0.0000	-2.79084701E-01	4.84282917E-09	(S)A-K
0.0000	-2.35666247E-02	2.06399014E-09	(S)A-N
0.0000	-9.03267155E-03	2.04606994E-09	(S)a'
0.0007	-3.27957563E-07	2.44383407E-10	(S)D-KK
0.0015	1.72344373E-05	2.52032162E-08	(S)D-KN
0.0019	-1.36843846E-05	2.55280649E-08	(S)D-NK
0.0002	7.76173237E-07	1.69695435E-10	(S)D-NN
0.0004	2.00348148E-06	7.26684827E-10	(S)d-N
0.0000	1.11224880E-06	3.86307168E-11	(S)d'
0.0316	-1.16532044E-10	3.68352644E-12	(S)H-KKK
0.2018	-1.28201343E-09	2.58683768E-10	(S)H-KNK
0.1862	1.69209828E-09	3.15067067E-10	(S)H-NNK
0.1817	-2.92964695E-10	5.32201688E-11	(S)H-NNN
0.2142	-3.41274164E-09	7.30964082E-10	(S)h-KN
0.0513	-8.53006032E-12	4.37310565E-13	(S)h-NN
0.1822	1.46153771E-10	2.66309408E-11	(S)h-N
0.0091	8.49483033E-12	7.76662443E-14	(S)h'

S-A FITTING FOR A MOLECULE WITH K = -0.5,
A TENDENCY = 10^{-2} IN THE ROTOR PART ONLY

Source	Number	Std. Dev.	Scaled
CALC	241	0.0000 Cm-1	0.0000
All	241	0.0011 MHz	0.0000
Ratio	Cm-1	Std. Dev.	
0.0000	1.31254905E+01	1.34671544E-09	A-K
0.0000	1.05638561E+01	5.84976600E-10	A-N
0.0000	9.37638615E-01	6.03431496E-10	a
0.0000	6.42736646E-05	4.02992133E-11	D-KK
0.0000	1.42862481E-04	5.09129556E-11	D-KN

0.0000	9.28574908E-05	1.59883987E-11	D-NN
0.0000	1.00000115E-04	1.60481683E-11	d-N
0.0000	4.57191046E-06	5.58646233E-12	d
0.0002	-2.00494131E-09	3.02041451E-13	H-KKK
0.0009	-6.34110598E-10	5.96278196E-13	H-KKN
0.0001	3.33698384E-09	4.53557866E-13	H-KNN
0.0002	-6.99054388E-10	1.05177307E-13	H-NNN
0.0066	-1.52924356E-11	1.01679081E-13	h-NN
0.0002	3.49862491E-10	5.55432423E-14	h-N
0.0007	1.53511179E-11	1.14905601E-14	h
0.0000	-2.79069161E-01	1.24698289E-08	(S)A-K
0.0000	-2.35710660E-02	5.16827033E-09	(S)A-N
0.0000	-9.06386039E-03	3.79349421E-09	(S)a'
0.0001	1.21910463E-05	7.60450130E-10	(S)D-KK
0.0001	-9.55782388E-05	7.70833546E-09	(S)D-KN
0.0001	8.43861978E-05	7.33780998E-09	(S)D-NK
0.0000	3.00012585E-06	7.10795076E-11	(S)D-NN
0.0001	3.11072200E-05	1.73067581E-09	(S)d-K
0.0000	2.00219792E-06	5.46100021E-11	(S)d-N
0.0728	-7.86840318E-10	5.72994517E-11	(S)H-KKK
0.0902	9.09014698E-10	8.20135943E-11	(S)H-KNK
0.2030	-1.23638556E-10	2.51005754E-11	(S)H-NNK
0.1184	-9.65356748E-10	1.14302693E-10	(S)h-KK
0.0070	-2.19841435E-09	1.53901764E-11	(S)h-KN

A-A FITTING FOR A MOLECULE WITH K = 0,
A TENDENCY = 10^{-2} IN THE ROTOR PART ONLY

Source	Number	Std. Dev.	Scaled
CALC	241	0.0000 Cm-1	0.0000
All	241	0.0001 MHz	0.0000
Ratio	Cm-1	Std. Dev.	
0.0000	1.31255551E+01	1.31435141E-10	A-K
0.0000	1.05638379E+01	4.94039599E-11	A-N
0.0000	2.18757818E+00	2.71110149E-11	a
0.0000	1.10003017E-04	5.26607663E-12	D-KK
0.0000	8.79982979E-05	4.28266660E-12	D-KN
0.0000	1.02000005E-04	5.66575307E-13	D-NN
0.0000	1.11996720E-04	4.88741912E-12	d-K
0.0000	1.00000457E-04	3.39715915E-13	d-N
0.0001	8.49340494E-10	1.20213602E-13	H-KKK
0.0001	-1.21312525E-09	1.77964962E-13	H-KKN
0.0002	3.63937494E-10	6.62765082E-14	H-KNN
0.0003	3.37742885E-10	1.08621293E-13	h-KK
0.0001	-4.56707347E-10	4.85914253E-14	h-KN
0.0000	-2.79069176E-01	1.42860819E-09	(S)A-K
0.0000	-2.35710579E-02	5.67470374E-10	(S)A-N
0.0000	-2.10927661E-02	3.61203678E-10	(S)a'
0.0000	1.11876699E-05	7.81476472E-11	(S)D-KK
0.0001	-1.80646924E-05	1.00713336E-09	(S)D-KN
0.0001	7.87838935E-06	9.89819058E-10	(S)D-NK
0.0000	3.00001397E-06	7.64248141E-12	(S)D-NN
0.0000	1.38267591E-05	7.74227630E-11	(S)d-K
0.0000	2.00046349E-06	5.18989792E-12	(S)d-N

0.0031	8.83372316E-10	2.69970634E-12	(S)H-KKK
0.0475	-8.08965098E-10	3.84444952E-11	(S)H-KKN
0.0807	-4.68349742E-10	3.78182247E-11	(S)H-KNK
0.0124	1.04121014E-09	1.29314431E-11	(S)H-KNN
0.0202	-6.47084851E-10	1.31005697E-11	(S)H-NNK
0.0072	3.27504735E-10	2.34581447E-12	(S)h-KK
0.0017	-4.61546908E-10	7.64989695E-13	(S)h-KN

A-S FITTING FOR A MOLECULE WITH K = 0,
A TENDENCY = 10^{-2} IN THE ROTOR PART ONLY

Source	Number	Std. Dev.	Scaled
CALC	241	0.0000 Cm-1	0.0000
All	241	0.0001 MHz	0.0000
Ratio	Cm-1	Std. Dev.	
0.0000	1.31255552E+01	1.34503748E-10	A-K
0.0000	1.05638378E+01	5.59771775E-11	A-N
0.0000	2.18757820E+00	4.75837836E-11	a
0.0000	1.10003041E-04	5.85786511E-12	D-KK
0.0000	8.79982497E-05	7.27733227E-12	D-KN
0.0000	1.02000015E-04	1.76873432E-12	D-NN
0.0000	1.11996738E-04	5.00537488E-12	d-K
0.0000	1.00000451E-04	1.27218256E-12	d-N
0.0001	8.49416703E-10	9.98720872E-14	H-KKK
0.0001	-1.21352988E-09	1.53322499E-13	H-KKN
0.0002	3.64379036E-10	7.89033732E-14	H-KNN
0.1331	-9.99090221E-14	1.33020072E-14	H-NNN
0.0003	3.37797638E-10	9.05907992E-14	h-KK
0.0001	-4.56988098E-10	4.99599198E-14	h-KN
0.2497	3.29434243E-14	8.22742393E-15	h-NN
0.0000	-2.79085292E-01	1.37484669E-09	(S)A-K
0.0000	-2.35664553E-02	5.76165848E-10	(S)A-N
0.0000	-2.10789026E-02	4.86284600E-10	(S)a'
0.0001	-5.98968245E-07	7.63713012E-11	(S)D-KK
0.0001	6.42529720E-06	7.92910136E-10	(S)D-KN
0.0003	-2.51928508E-06	8.08708270E-10	(S)D-NK
0.0000	6.92641749E-07	2.04762744E-11	(S)D-NN
0.0000	2.00015394E-06	1.84335468E-11	(S)d-N
0.0000	1.15371835E-06	6.81778516E-12	(S)d'
0.0128	-6.85408907E-11	8.80591758E-13	(S)H-KKK
0.5838	-5.06919012E-11	2.95945590E-11	(S)H-KKN
0.8828	-3.66331219E-11	3.23384216E-11	(S)H-KNK
0.0562	1.93714041E-10	1.08890975E-11	(S)H-NNK
0.0489	-3.77467868E-11	1.84660273E-12	(S)H-NNN
0.0641	-1.70486962E-10	1.09235397E-11	(S)h-KN
0.0755	1.42450561E-12	1.07542525E-13	(S)h-NN
0.0494	1.88802793E-11	9.32431812E-13	(S)h-N
0.0135	-1.38435281E-12	1.87021676E-14	(S)h'

S-S FITTING FOR A MOLECULE WITH K = 0,
A TENDENCY = 10^{-2} IN THE ROTOR PART ONLY

Source	Number	Std. Dev.	Scaled
CALC	241	0.0000 Cm-1	0.0000

All	241	0.0003 MHz	0.0000
Ratio	Cm-1	Std. Dev.	
0.0000	1.31256579E+01	3.55152043E-10	A-K
0.0000	1.05638085E+01	1.48647587E-10	A-N
0.0000	2.18749019E+00	1.25675072E-10	a
0.0000	-1.66760997E-05	1.26777445E-11	D-KK
0.0000	-1.99996511E-04	1.53259519E-11	D-KN
0.0000	-8.33328787E-05	4.20597155E-12	D-NN
0.0000	-9.99998325E-05	3.37212894E-12	d-N
0.0000	-9.33295712E-06	1.11126251E-12	d
0.0001	-1.58936596E-09	1.04443399E-13	H-KKK
0.0003	-6.44639814E-10	2.03778552E-13	H-KKN
0.0001	2.81778961E-09	1.48082470E-13	H-KNN
0.0000	-5.83285493E-10	2.90321477E-14	H-NNN
0.0010	-2.17482168E-11	2.16165705E-14	h-NN
0.0000	2.91506820E-10	1.10550027E-14	h-N
0.0001	2.17682213E-11	2.32059814E-15	h
0.0000	-2.79084101E-01	3.65809932E-09	(S)A-K
0.0000	-2.35667956E-02	1.53895903E-09	(S)A-N
0.0000	-2.10789056E-02	1.30069423E-09	(S)a'
0.0007	2.74448721E-07	2.03395827E-10	(S)D-KK
0.0003	4.38333582E-06	1.38364730E-09	(S)D-KN
0.0009	-1.52032746E-06	1.41006824E-09	(S)D-NK
0.0001	8.62649394E-07	5.26067218E-11	(S)D-NN
0.0000	1.99992779E-06	4.01967112E-11	(S)d-N
0.0000	1.06865506E-06	1.76302593E-11	(S)d'
0.2902	7.82969925E-12	2.27184849E-12	(S)H-KKK
0.4188	1.85319541E-10	7.76056558E-11	(S)H-KKN
0.8063	-9.46650394E-11	7.63289989E-11	(S)H-KNK
0.0210	-1.19260809E-10	2.50876382E-12	(S)H-NNK
0.0201	2.08761305E-11	4.19014413E-13	(S)H-NNN
0.0378	7.61607990E-12	2.87683187E-13	(S)h-NN
0.0175	-1.04153803E-11	1.82214791E-13	(S)h-N
0.0063	-7.52610333E-12	4.73353686E-14	(S)h'

S-A FITTING FOR A MOLECULE WITH K = 0,
A TENDENCY = 10^{-2} IN THE ROTOR PART ONLY

Source	Number	Std. Dev.	Scaled
CALC	241	0.0000 Cm-1	0.0000
All	241	0.0003 MHz	0.0000
Ratio	Cm-1	Std. Dev.	
0.0000	1.31256577E+01	3.60158013E-10	A-K
0.0000	1.05638085E+01	1.49462622E-10	A-N
0.0000	2.18749017E+00	1.26015472E-10	a
0.0000	-1.66760849E-05	1.26187005E-11	D-KK
0.0000	-1.99996531E-04	1.53772071E-11	D-KN
0.0000	-8.33328772E-05	4.22993644E-12	D-NN
0.0000	-9.99998319E-05	3.38289220E-12	d-N
0.0000	-9.33295698E-06	1.10518504E-12	d
0.0001	-1.58935840E-09	1.04207336E-13	H-KKK
0.0003	-6.44653043E-10	2.03248608E-13	H-KKN
0.0001	2.81780537E-09	1.48234965E-13	H-KNN
0.0001	-5.83289607E-10	2.92173473E-14	H-NNN

0.0010	-2.17515802E-11	2.17015542E-14	h-NN
0.0000	2.91506492E-10	1.09967195E-14	h-N
0.0001	2.17684029E-11	2.31723655E-15	h
0.0000	-2.79069173E-01	3.15130600E-09	(S)A-K
0.0000	-2.35710592E-02	1.25107604E-09	(S)A-N
0.0000	-2.10917496E-02	7.97427621E-10	(S)a'
0.0000	1.11895880E-05	1.71131784E-10	(S)D-KK
0.0001	-1.83026295E-05	2.11271318E-09	(S)D-KN
0.0003	8.11328098E-06	2.07951182E-09	(S)D-NK
0.0000	3.00001412E-06	1.68739190E-11	(S)D-NN
0.0000	1.28099680E-05	1.70786363E-10	(S)d-K
0.0000	1.99968803E-06	1.14553164E-11	(S)d-N
0.0328	1.81705970E-10	5.95834335E-12	(S)H-KKK
0.1047	7.87378124E-10	8.24439197E-11	(S)H-KKN
0.0778	-1.03980356E-09	8.09354718E-11	(S)H-KNK
0.0267	-9.48894927E-10	2.53073498E-11	(S)H-KNN
0.0252	1.01982158E-09	2.57200514E-11	(S)H-NNK
0.0605	8.61471884E-11	5.20797265E-12	(S)h-KK
0.0054	3.12370504E-10	1.68580053E-12	(S)h-KN

A-A FITTING FOR A MOLECULE WITH K = -0.25,
A TENDENCY = 10^{-2} IN THE ROTOR PART ONLY

Source	Number	Std. Dev.	Scaled
CALC	241	0.0000 Cm-1	0.0000
All	241	0.0001 MHz	0.0000
Ratio	Cm-1	Std. Dev.	
0.0000	1.31255269E+01	1.48435618E-09	A-K
0.0000	1.05638459E+01	6.07322894E-10	A-N
0.0000	1.51450283E+00	2.09200091E-10	a
0.0000	-1.09995507E-04	5.13690132E-11	D-KK
0.0000	-8.80024183E-05	5.54106517E-11	D-KN
0.0000	-1.02000036E-04	9.53070632E-12	D-NN
0.0000	-1.17337887E-04	7.13637194E-11	d-K
0.0000	-9.99989578E-05	2.16832625E-12	d-N
0.0020	1.25335523E-09	2.49566230E-12	H-KKK
0.0020	-1.79051773E-09	3.56857969E-12	H-KKN
0.0020	5.37110592E-10	1.09875726E-12	H-KNN
0.0055	5.72225212E-10	3.15285848E-12	h-KK
0.0004	-1.03813912E-09	4.57678694E-13	h-KN
0.0000	-2.79069128E-01	8.72612898E-09	(S)A-K
0.0000	-2.35710757E-02	3.73761386E-09	(S)A-N
0.0000	-1.46120087E-02	1.90584175E-09	(S)a'
0.0001	1.14299311E-05	6.70818357E-10	(S)D-KK
0.0001	-3.73194738E-05	2.52711681E-09	(S)D-KN
0.0001	2.68868361E-05	2.19456141E-09	(S)D-NK
0.0000	3.00007073E-06	1.27516027E-10	(S)D-NN
0.0001	1.94903604E-05	1.01465129E-09	(S)d-K
0.0000	1.99875752E-06	6.43738624E-11	(S)d-N
0.0358	-1.53493236E-09	5.49335284E-11	(S)H-KKK
0.0476	2.25383259E-09	1.07198707E-10	(S)H-KKN
0.8936	-4.45525900E-11	3.98144061E-11	(S)H-KNK
0.0066	-3.30890671E-09	2.18206233E-11	(S)H-KNN
0.0073	2.62378648E-09	1.92843667E-11	(S)H-NNK

0.2519	5.16486937E-12	1.30128000E-12	(S)H-NNN
0.0982	-6.92704373E-10	6.80580007E-11	(S)h-KK
0.0095	1.22213893E-09	1.16499213E-11	(S)h-KN

A-S FITTING FOR A MOLECULE WITH K = -0.25,
A TENDENCY = 10^{-2} IN THE ROTOR PART ONLY

Source	Number	Std. Dev.	Scaled
CALC	241	0.0000 Cm-1	0.0000
All	241	0.0001 MHz	0.0000
Ratio	Cm-1	Std. Dev.	
0.0000	1.31255272E+01	1.57504340E-09	A-K
0.0000	1.05638458E+01	6.41869261E-10	A-N
0.0000	1.51450285E+00	4.96015502E-10	a
0.0000	-1.09995550E-04	5.39688908E-11	D-KK
0.0000	-8.80023725E-05	5.89545594E-11	D-KN
0.0000	-1.02000038E-04	1.01800557E-11	D-NN
0.0000	-1.17337868E-04	7.48889400E-11	d-K
0.0000	-9.99989541E-05	5.40847025E-12	d-N
0.0021	1.25158607E-09	2.64483230E-12	H-KKK
0.0021	-1.78800743E-09	3.77397596E-12	H-KKN
0.0022	5.36340290E-10	1.15700855E-12	H-KNN
0.0061	5.70630652E-10	3.45586293E-12	h-KK
0.0005	-1.03835501E-09	4.69172704E-13	h-KN
0.0000	-2.79084845E-01	9.17590142E-09	(S)A-K
0.0000	-2.35665865E-02	3.91218178E-09	(S)A-N
0.0000	-1.45924656E-02	3.34490245E-09	(S)a'
0.0015	-3.49104946E-07	5.30398445E-10	(S)D-KK
0.0002	9.00049419E-06	1.69428747E-09	(S)D-KN
0.0003	-5.40059081E-06	1.53088517E-09	(S)D-NK
0.0002	7.49420499E-07	1.62249373E-10	(S)D-NN
0.0000	1.99916053E-06	8.52704560E-11	(S)d-N
0.0000	1.12521924E-06	5.31595188E-11	(S)d'
0.0409	6.79313364E-10	2.77986758E-11	(S)H-KKN
0.1269	-2.23847066E-10	2.84161941E-11	(S)H-KNK
0.0316	-5.57614997E-10	1.76334728E-11	(S)H-NNK
0.0345	9.72251783E-11	3.35507313E-12	(S)H-NNN
0.0331	8.52285907E-10	2.82360790E-11	(S)h-KN
0.5939	-1.60666398E-12	9.54243035E-13	(S)h-NN
0.0356	-4.60454801E-11	1.64106501E-12	(S)h-N
0.3960	8.86251907E-13	3.50942418E-13	(S)h'

S-S FITTING FOR A MOLECULE WITH K = -0.25,
A TENDENCY = 10^{-2} IN THE ROTOR PART ONLY

Source	Number	Std. Dev.	Scaled
CALC	241	0.0000 Cm-1	0.0000
All	241	0.0001 MHz	0.0000
Ratio	Cm-1	Std. Dev.	
0.0000	1.31256220E+01	1.64134654E-09	A-K
0.0000	1.05638188E+01	7.08492070E-10	A-N
0.0000	1.51438552E+00	6.44532063E-10	a
0.0000	-4.23175078E-05	3.74895616E-11	D-KK
0.0000	-1.69227779E-04	3.71544018E-11	D-KN

0.0000	-8.84608730E-05	6.96083350E-12	D-NN
0.0000	-9.99998493E-05	5.42425029E-12	d-N
0.0000	-6.76887973E-06	4.19203037E-12	d
0.0003	-1.77023423E-09	5.33572414E-13	H-KKK
0.0012	-7.38524467E-10	8.63253569E-13	H-KKN
0.0001	3.16253114E-09	4.56561017E-13	H-KNN
0.0001	-6.53576443E-10	8.02343432E-14	H-NNN
0.0036	-1.84463641E-11	6.67053003E-14	h-NN
0.0001	3.26742675E-10	3.34927600E-14	h-N
0.0009	1.84119595E-11	1.60208467E-14	h
0.0000	-2.79083872E-01	9.07699714E-09	(S)A-K
0.0000	-2.35668581E-02	3.95279130E-09	(S)A-N
0.0000	-1.45924812E-02	3.57638529E-09	(S)a'
0.0011	4.64453058E-07	5.29822530E-10	(S)D-KK
0.0003	5.29913744E-06	1.68318448E-09	(S)D-KN
0.0006	-2.66487866E-06	1.49725584E-09	(S)D-NK
0.0002	9.02718392E-07	2.21120070E-10	(S)D-NN
0.0001	1.99953888E-06	1.97490095E-10	(S)d-N
0.0001	1.04838514E-06	5.85951966E-11	(S)d'
0.0446	2.53881407E-10	1.13202617E-11	(S)H-KKK
0.2929	-9.28644754E-11	2.72018014E-11	(S)H-KKN
0.8028	3.61395206E-11	2.90136647E-11	(S)H-KNK
0.0686	-2.48199076E-10	1.70358763E-11	(S)H-NNK
0.0597	5.80436339E-11	3.46641405E-12	(S)H-NNN
0.1221	2.44646523E-10	2.98761831E-11	(S)h-KN
0.3032	7.69437193E-12	2.33300337E-12	(S)h-NN
0.0599	-3.11154551E-11	1.86489493E-12	(S)h-N
0.0485	-7.10041490E-12	3.44266095E-13	(S)h'

S-A FITTING FOR A MOLECULE WITH K = -0.25,
A TENDENCY = 10^{-2} IN THE ROTOR PART ONLY

Source	Number	Std. Dev.	Scaled
CALC	241	0.0000 Cm-1	0.0000
All	241	0.0001 MHz	0.0000
Ratio	Cm-1	Std. Dev.	
0.0000	1.31256217E+01	1.61606545E-09	A-K
0.0000	1.05638188E+01	7.05698214E-10	A-N
0.0000	1.51438549E+00	3.29278560E-10	a
0.0000	-4.23174590E-05	3.80426722E-11	D-KK
0.0000	-1.69227839E-04	3.76904872E-11	D-KN
0.0000	-8.84608671E-05	7.05958245E-12	D-NN
0.0000	-9.99998480E-05	5.50103340E-12	d-N
0.0000	-6.76888092E-06	4.24745474E-12	d
0.0003	-1.77032293E-09	5.41406138E-13	H-KKK
0.0012	-7.38596411E-10	8.75065267E-13	H-KKN
0.0001	3.16270098E-09	4.55641461E-13	H-KNN
0.0001	-6.53602292E-10	7.91916155E-14	H-NNN
0.0013	-1.84291732E-11	2.34746090E-14	h-NN
0.0001	3.26758826E-10	3.36970714E-14	h-N
0.0009	1.84125894E-11	1.57706689E-14	h
0.0000	-2.79069229E-01	9.13407225E-09	(S)A-K
0.0000	-2.35710400E-02	3.98225713E-09	(S)A-N
0.0000	-1.46106804E-02	3.07984324E-09	(S)a'

0.0001	1.14452983E-05	8.02774252E-10	(S)D-KK
0.0001	-3.78500015E-05	2.89370499E-09	(S)D-KN
0.0001	2.74066907E-05	2.31768766E-09	(S)D-NK
0.0001	2.99963395E-06	2.47935939E-10	(S)D-NN
0.0001	1.81517748E-05	1.14290107E-09	(S)d-K
0.0000	1.99917300E-06	6.92829556E-11	(S)d-N
0.0952	6.11412551E-10	5.82148633E-11	(S)H-KKK
0.1667	6.85945498E-10	1.14375286E-10	(S)H-KKN
0.0270	-1.54791686E-09	4.17918518E-11	(S)H-KNK
0.0093	-2.73554221E-09	2.53297842E-11	(S)H-KNN
0.0066	2.99835468E-09	1.97373484E-11	(S)H-NNK
0.6737	-4.53054042E-12	3.05224006E-12	(S)H-NNN
0.2403	2.99222229E-10	7.19091662E-11	(S)h-KK
0.0200	7.20294880E-10	1.43963142E-11	(S)h-KN

A-A FITTING FOR A MOLECULE WITH K = -0.75,
A TENDENCY = 10^{-2} IN THE ROTOR PART ONLY

Source	Number	Std. Dev.	Scaled
CALC	241	0.0000 Cm-1	0.0000
All	241	0.0017 MHz	0.0000
Ratio	Cm-1	Std. Dev.	
0.0000	1.31255242E+01	2.14498832E-08	A-K
0.0000	1.05638459E+01	7.76552573E-09	A-N
0.0000	4.37577917E-01	6.33917262E-09	a
0.0000	-1.09986948E-04	1.12099020E-09	D-KK
0.0000	-8.80053947E-05	1.06681901E-09	D-KN
0.0000	-1.02000906E-04	1.77952188E-10	D-NN
0.0000	-1.59967319E-04	5.91719872E-09	d-K
0.0000	-9.99858286E-05	4.62434327E-11	d-N
0.0306	3.88319852E-09	1.18697501E-10	H-KKK
0.0299	-5.57939332E-09	1.66752588E-10	H-KKN
0.0286	1.69003530E-09	4.82642038E-11	H-KNN
0.1951	3.74384106E-12	7.30527827E-13	H-NNN
0.4280	-1.15626017E-09	4.94914957E-10	h-KK
0.0022	-1.41474304E-08	3.15593214E-11	h-KN
0.0000	-2.79068534E-01	1.21746677E-07	(S)A-K
0.0000	-2.35713844E-02	4.99306729E-08	(S)A-N
0.0000	-4.27602247E-03	8.97985560E-08	(S)a'
0.0010	1.67452433E-05	1.73164039E-08	(S)D-KK
0.0015	-4.45661467E-04	6.59503573E-07	(S)D-KN
0.0015	4.29898626E-04	6.44673658E-07	(S)D-NK
0.0009	3.00780247E-06	2.63699606E-09	(S)D-NN
0.0016	6.16681516E-05	9.70844780E-08	(S)d-K
0.0006	1.98322687E-06	1.27000767E-09	(S)d-N
0.2828	-1.01960490E-08	2.88388263E-09	(S)H-KKK
0.1408	-3.96203627E-07	5.57662444E-08	(S)H-KKN
0.1387	3.79986461E-07	5.26973066E-08	(S)H-KNK
0.3829	-5.29777050E-08	2.02835274E-08	(S)H-KNN
0.3381	5.91234703E-08	1.99868403E-08	(S)H-NNK
0.1789	5.67127790E-08	1.01451014E-08	(S)h-KK
0.0369	2.02398932E-08	7.47031578E-10	(S)h-KN

A-S FITTING FOR A MOLECULE WITH K = -0.75,
A TENDENCY = 10^{-2} IN THE ROTOR PART ONLY

Source	Number	Std. Dev.	Scaled
CALC	241	0.0000 Cm-1	0.0000
All	241	0.0008 MHz	0.0000
Ratio	Cm-1	Std. Dev.	
0.0000	1.31255274E+01	1.17505895E-08	A-K
0.0000	1.05638458E+01	5.03029191E-09	A-N
0.0000	4.37578073E-01	3.43578062E-09	a
0.0000	-1.09986187E-04	4.27789883E-10	D-KK
0.0000	-8.80066860E-05	4.81748961E-10	D-KN
0.0000	-1.02000241E-04	8.80758599E-11	D-NN
0.0000	-1.60031211E-04	2.81526318E-09	d-K
0.0000	-9.99863737E-05	2.77847416E-11	d-N
0.0045	4.19019586E-09	1.88003391E-11	H-KKK
0.0045	-5.98543095E-09	2.69751737E-11	H-KKN
0.0051	1.78025662E-09	9.06412106E-12	H-KNN
0.1538	5.05740396E-12	7.77953345E-13	H-NNN
0.1117	7.16679207E-10	8.00406670E-11	h-KK
0.0018	-1.36548834E-08	2.46190371E-11	h-KN
0.0000	-2.79083731E-01	6.86373993E-08	(S)A-K
0.0000	-2.35668991E-02	2.88546385E-08	(S)A-N
0.0000	-4.21420600E-03	1.36767161E-08	(S)a'
0.0190	2.00446705E-07	3.81228411E-09	(S)D-KK
0.0028	3.01964112E-05	8.32437994E-08	(S)D-KN
0.0030	-2.72797298E-05	8.17633173E-08	(S)D-NK
0.0019	9.08362906E-07	1.73431566E-09	(S)D-NN
0.0056	1.68170843E-06	9.42766141E-09	(S)d-N
0.0005	1.04173123E-06	5.53942762E-10	(S)d'
0.2194	-5.83418981E-10	1.28025353E-10	(S)H-KKK
0.1026	-3.06900248E-08	3.14979494E-09	(S)H-KKN
0.0508	8.25844156E-08	4.19418373E-09	(S)H-KNK
0.0291	-6.11612248E-08	1.78284122E-09	(S)H-NNK
0.0298	1.01422949E-08	3.02610417E-10	(S)H-NNN
0.0293	3.17447200E-07	9.31351710E-09	(S)h-KN
0.0299	-5.14374998E-09	1.53853794E-10	(S)h-N
0.0788	9.05387206E-12	7.13896755E-13	(S)h'

S-S FITTING FOR A MOLECULE WITH K = -0.75,
A TENDENCY = 10^{-2} IN THE ROTOR PART ONLY

Source	Number	Std. Dev.	Scaled
CALC	241	0.0000 Cm-1	0.0000
All	241	0.0003 MHz	0.0000
Ratio	Cm-1	Std. Dev.	
0.0000	1.31255646E+01	4.05295125E-09	A-K
0.0000	1.05638352E+01	1.66540169E-09	A-N
0.0000	4.37418034E-01	7.87949802E-10	a
0.0000	-8.33469280E-05	1.76971361E-10	D-KK
0.0000	-1.19994383E-04	2.33186624E-10	D-KN
0.0000	-9.66661760E-05	4.45998318E-11	D-NN
0.0000	-9.99999024E-05	1.39104157E-11	d-N
0.0000	-2.66614331E-06	2.22064576E-11	d
0.0004	-2.35769265E-09	8.47495119E-13	H-KKK

0.0079	-3.14371895E-10	2.48717111E-12	H-KKN
0.0007	3.40939971E-09	2.33749442E-12	H-KNN
0.0005	-7.36742306E-10	3.77774635E-13	H-NNN
0.0049	-1.14346598E-11	5.57666744E-14	h-NN
0.0006	3.68302391E-10	2.08971067E-13	h-N
0.0037	1.15585605E-11	4.23480868E-14	h
0.0000	-2.79083354E-01	2.38892990E-08	(S)A-K
0.0000	-2.35670091E-02	9.62950734E-09	(S)A-N
0.0000	-4.21418353E-03	6.65534865E-09	(S)a'
0.0026	6.92994592E-07	1.81022510E-09	(S)D-KK
0.0018	1.41747718E-05	2.61567396E-08	(S)D-KN
0.0022	-1.18412769E-05	2.63034170E-08	(S)D-NK
0.0008	9.72808880E-07	7.75886557E-10	(S)D-NN
0.0033	2.02188878E-06	6.69019686E-09	(S)d-N
0.0002	1.01385052E-06	2.18926425E-10	(S)d'
0.1638	2.27310265E-10	3.72376160E-11	(S)H-KKK
0.1640	1.00579059E-08	1.64920684E-09	(S)H-KKN
0.1908	-1.38455042E-08	2.64132650E-09	(S)H-KNK
0.3069	4.25083767E-09	1.30469350E-09	(S)H-NNK
0.3186	-6.88782767E-10	2.19464180E-10	(S)H-NNN
0.3088	-2.16466430E-08	6.68490386E-09	(S)h-KN
0.3215	3.43766805E-10	1.10536623E-10	(S)h-N
0.1739	-5.06521421E-12	8.81035377E-13	(S)h'

S-A FITTING FOR A MOLECULE WITH K = -0.75,
A TENDENCY = 10^{-2} IN THE ROTOR PART ONLY

Source	Number	Std. Dev.	Scaled
CALC	241	0.0000 Cm-1	0.0000
All	241	0.0004 MHz	0.0000
Ratio	Cm-1	Std. Dev.	
0.0000	1.31255616E+01	5.16971770E-09	A-K
0.0000	1.05638352E+01	1.90324575E-09	A-N
0.0000	4.37417958E-01	1.30641325E-09	a
0.0000	-8.33450439E-05	1.30652226E-10	D-KK
0.0000	-1.19995286E-04	1.50223116E-10	D-KN
0.0000	-9.66659648E-05	2.22352326E-11	D-NN
0.0000	-9.99998142E-05	2.30766010E-11	d-N
0.0000	-2.66623608E-06	1.88596657E-11	d
0.0007	-2.35872228E-09	1.66095398E-12	H-KKK
0.0065	-3.48191793E-10	2.24895184E-12	H-KKN
0.0003	3.44682493E-09	1.12005068E-12	H-KNN
0.0002	-7.38780979E-10	1.75639188E-13	H-NNN
0.0080	-1.16654518E-11	9.37458922E-14	h-NN
0.0003	3.69327630E-10	1.22301810E-13	h-N
0.0033	1.18624559E-11	3.97024619E-14	h
0.0000	-2.79069348E-01	2.98174364E-08	(S)A-K
0.0000	-2.35710660E-02	1.22286967E-08	(S)A-N
0.0000	-4.27517802E-03	2.28718364E-08	(S)a'
0.0002	1.68516589E-05	4.13175547E-09	(S)D-KK
0.0003	-4.53981339E-04	1.55058857E-07	(S)D-KN
0.0003	4.38133542E-04	1.51375368E-07	(S)D-NK
0.0002	2.99901708E-06	6.45695247E-10	(S)D-NN
0.0003	6.08114258E-05	2.08397864E-08	(S)d-K

0.0002	1.98665871E-06	3.30132303E-10	(S)d-N
0.3725	1.26378755E-09	4.70748886E-10	(S)H-KKK
0.1328	-4.75519145E-09	6.31285190E-10	(S)H-KKN
0.0219	-1.29540675E-07	2.83746488E-09	(S)H-KNN
0.0225	1.33102206E-07	2.99461613E-09	(S)H-NNK
0.7192	2.71295852E-09	1.95122321E-09	(S)h-KK
0.0135	1.31832462E-08	1.78550135E-10	(S)h-KN

A-A FITTING FOR A MOLECULE WITH K = -0.9,
A TENDENCY = 10^{-2} IN THE ROTOR PART ONLY

Source	Number	Std. Dev.	Scaled
CALC	241	0.0000 Cm-1	0.0000
All	241	0.0735 MHz	0.0000
Ratio	Cm-1	Std. Dev.	
0.0000	1.31255049E+01	2.19005457E-07	A-K
0.0000	1.05638460E+01	3.12738088E-08	A-N
0.0000	1.68382910E-01	5.24212747E-08	a
0.0000	-1.10044287E-04	3.72580864E-09	D-KK
0.0001	-8.77787081E-05	5.33268659E-09	D-KN
0.0000	-1.02001083E-04	3.74285065E-10	D-NN
0.0002	-2.55572190E-04	4.53165628E-08	d-K
0.0000	-9.98918423E-05	5.30336942E-10	d-N
0.0009	1.60984012E-08	1.49026873E-11	H-KKK
0.0016	-2.32594413E-08	3.60878563E-11	H-KKN
0.0038	7.01808504E-09	2.66802389E-11	H-KNN
0.0042	-1.05224728E-07	4.46226662E-10	h-KN
0.0000	-2.79069677E-01	8.09800442E-07	(S)A-K
0.0000	-2.35711740E-02	3.42333186E-07	(S)A-N
0.0005	-1.78041139E-03	8.17391707E-07	(S)a'
0.0079	5.47801662E-05	4.32228001E-07	(S)D-KK
0.0094	-3.37608307E-03	3.18774390E-05	(S)D-KN
0.0095	3.32254750E-03	3.14567086E-05	(S)D-NK
0.0017	3.00211974E-06	5.16084943E-09	(S)D-NN
0.0050	1.60416349E-04	8.02874021E-07	(S)d-K
0.0039	1.89327056E-06	7.32111950E-09	(S)d-N
0.1649	-3.21885798E-08	5.30839680E-09	(S)H-KKK
0.0531	-2.16520831E-07	1.14918816E-08	(S)H-KNK
0.0270	2.48423961E-07	6.71249070E-09	(S)H-KNN
0.8547	-7.95372480E-08	6.79790425E-08	(S)h-KK
0.0541	1.14062177E-07	6.17582093E-09	(S)h-KN

A-S FITTING FOR A MOLECULE WITH K = -0.9,
A TENDENCY = 10^{-2} IN THE ROTOR PART ONLY

Source	Number	Std. Dev.	Scaled
CALC	241	0.0000 Cm-1	0.0000
All	241	0.0657 MHz	0.0000
Ratio	Cm-1	Std. Dev.	
0.0000	1.31255265E+01	7.42676308E-08	A-K
0.0000	1.05638461E+01	3.28607695E-08	A-N
0.0000	1.68383602E-01	8.42464417E-08	a
0.0000	-1.09921493E-04	4.94887239E-09	D-KK
0.0001	-8.80091162E-05	5.54826340E-09	D-KN

0.0000	-1.02008320E-04	1.19231406E-09	D-NN
0.0003	-2.55991310E-04	7.07011278E-08	d-K
0.0000	-9.98993313E-05	1.42322325E-09	d-N
0.0139	1.69319173E-08	2.35502489E-10	H-KKK
0.0138	-2.41524667E-08	3.33226695E-10	H-KKN
0.0159	7.06181983E-09	1.12447434E-10	H-KNN
0.1602	6.12693825E-11	9.81649887E-12	H-NNN
0.2744	1.09747010E-08	3.01091770E-09	h-KK
0.0067	-1.01826586E-07	6.86265413E-10	h-KN
0.5859	1.36834995E-11	8.01652138E-12	h-NN
0.0000	-2.79084123E-01	9.29742241E-07	(S)A-K
0.0000	-2.35665070E-02	3.84804458E-07	(S)A-N
0.0002	-1.61963857E-03	2.44368649E-07	(S)a'
0.0487	7.35589454E-07	3.58291069E-08	(S)D-KK
0.0225	2.32328897E-06	5.22466341E-08	(S)D-NK
0.0159	9.27108226E-07	1.47026560E-08	(S)D-NN
0.0530	2.28899704E-06	1.21323948E-07	(S)d-N
0.0069	1.03175393E-06	7.13581269E-09	(S)d'
0.1136	-3.51759533E-08	3.99525269E-09	(S)H-KKK
0.1036	2.91152409E-06	3.01615189E-07	(S)H-KKN
0.1039	-2.89449757E-06	3.00627951E-07	(S)H-KNK
0.4126	2.15026714E-08	8.87268572E-09	(S)H-NNK
0.4179	-3.21070287E-09	1.34177722E-09	(S)H-NNN
0.4177	-2.89561249E-07	1.20955912E-07	(S)h-KN
0.4200	1.66747786E-09	7.00331789E-10	(S)h-N
0.9361	1.64872956E-11	1.54338382E-11	(S)h'

S-S FITTING FOR A MOLECULE WITH K = -0.9,
A TENDENCY = 10^{-2} IN THE ROTOR PART ONLY

All	241	0.0013 MHz	0.0000
Ratio	Cm-1	Std. Dev.	
0.0000	1.31255506E+01	1.62566215E-09	A-K
0.0000	1.05638393E+01	6.42458854E-10	A-N
0.0000	1.68127614E-01	9.19715678E-10	a
0.0000	-9.36116301E-05	6.13317160E-11	D-KK
0.0000	-1.07683943E-04	5.08360307E-11	D-KN
0.0000	-9.87178115E-05	1.73541593E-11	D-NN
0.0000	-9.99999136E-05	2.47551538E-11	d-N
0.0000	-1.64031627E-06	8.18515864E-12	d
0.0001	-2.54081043E-09	2.58883471E-13	H-KKK
0.0039	-1.35746296E-10	5.22779730E-13	H-KKN
0.0001	3.43167653E-09	4.24516922E-13	H-KNN
0.0001	-7.53842024E-10	1.12234035E-13	H-NNN
0.0169	-9.35856702E-12	1.57770971E-13	h-NN
0.0002	3.76763923E-10	8.24086435E-14	h-N
0.0016	9.26500860E-12	1.51272460E-14	h
0.0000	-2.79083195E-01	2.02620802E-08	(S)A-K
0.0000	-2.35670668E-02	8.02006190E-09	(S)A-N
0.0000	-1.61960641E-03	8.61378972E-09	(S)a'
0.0015	7.35853300E-05	1.12812537E-07	(S)D-KN
0.0016	-7.05747485E-05	1.12917172E-07	(S)D-NK
0.0003	9.90100726E-07	3.28821056E-10	(S)D-NN
0.0027	1.99387785E-06	5.47998396E-09	(S)d-N

0.0002	1.00493480E-06	1.80058491E-10	(S)d'
0.0086	1.11216834E-08	9.52059755E-11	(S)H-KKK
0.0086	-8.38521633E-07	7.22253967E-09	(S)H-KKN
0.0087	8.27731932E-07	7.20072576E-09	(S)H-KNK
0.9021	-4.10334090E-10	3.70182472E-10	(S)H-NNK
0.7637	8.15682130E-11	6.22975438E-11	(S)H-NNN
0.9324	5.85019960E-09	5.45472461E-09	(S)h-KN
0.2089	9.30498753E-12	1.94424356E-12	(S)h-NN
0.7798	-4.05195142E-11	3.15977776E-11	(S)h-N
0.0419	-7.40654574E-12	3.10584675E-13	(S)h'

S-A FITTING FOR A MOLECULE WITH K = -0.9,
A TENDENCY = 10^{-2} IN THE ROTOR PART ONLY

Source	Number	Std. Dev.	Scaled
CALC	241	0.0000 Cm-1	0.0000
All	241	0.2014 MHz	0.0000
Ratio	Cm-1	Std. Dev.	
0.0000	1.31255502E+01	2.26753931E-07	A-K
0.0000	1.05638393E+01	1.00341730E-07	A-N
0.0000	1.68127681E-01	6.00573612E-08	a
0.0002	-9.36271373E-05	1.43630547E-08	D-KK
0.0001	-1.07722029E-04	1.41209049E-08	D-KN
0.0000	-9.87178757E-05	2.70620588E-09	D-NN
0.0000	-1.00001820E-04	6.55224772E-10	d-N
0.0008	-1.64128131E-06	1.27719460E-09	d
0.0179	-2.50950082E-09	4.48348603E-11	H-KKK
0.5657	-1.57416686E-10	8.90432631E-11	H-KKN
0.0212	3.56142430E-09	7.56264704E-11	H-KNN
0.0230	-7.58433894E-10	1.74776162E-11	H-NNN
0.0335	3.84317482E-10	1.28631649E-11	h-N
0.2583	9.14266042E-12	2.36148047E-12	h
0.0000	-2.79068785E-01	2.66549547E-06	(S)A-K
0.0000	-2.35686429E-02	1.08350449E-06	(S)A-N
0.0024	-1.80423449E-03	4.36919516E-06	(S)a'
0.0315	8.05759646E-06	2.53615188E-07	(S)D-KK
0.0383	-7.95163234E-06	3.04406324E-07	(S)D-NK
0.0178	2.70321213E-06	4.82437191E-08	(S)D-NN
0.0234	1.94219450E-04	4.53762148E-06	(S)d-K
0.0193	1.66254534E-06	3.20863129E-08	(S)d-N
0.0369	-6.21739275E-07	2.29261972E-08	(S)H-KKK
0.1941	-5.36743694E-06	1.04167356E-06	(S)H-KKN
0.1640	6.31937595E-06	1.03637019E-06	(S)H-KNK
0.2777	-2.64960050E-06	7.35898684E-07	(S)H-KNN
0.3167	2.31756047E-06	7.33945702E-07	(S)H-NNK
0.1509	2.87355550E-09	4.33721380E-10	(S)H-NNN
0.0359	-8.07900122E-06	2.90333423E-07	(S)h-KK
0.1111	2.82665551E-07	3.13950707E-08	(S)h-KN

S-S FITTING FOR A MOLECULE WITH K = -0.99,
A TENDENCY = 10^{-2} IN THE ROTOR PART ONLY

Source	Number	Std. Dev.	Scaled
CALC	241	0.0000 Cm-1	0.0000

All	241	0.0007 MHz	0.0000
Ratio	Cm-1	Std. Dev.	
0.0000	1.31255420E+01	7.99545818E-10	A-K
0.0000	1.05638416E+01	3.55240309E-10	A-N
0.0000	1.63480400E-02	5.54230714E-10	a
0.0000	-9.93885187E-05	2.09404362E-11	D-KK
0.0000	-1.00745413E-04	2.77948025E-11	D-KN
0.0000	-9.98742073E-05	9.55930464E-12	D-NN
0.0000	-9.99999467E-05	1.54497491E-11	d-N
0.0000	-1.06210622E-06	4.47522948E-12	d
0.0001	-2.66538728E-09	1.38449136E-13	H-KKK
0.2588	-1.08455891E-12	2.80682297E-13	H-KKN
0.0001	3.42996027E-09	2.30586361E-13	H-KNN
0.0001	-7.62322406E-10	6.15237832E-14	H-NNN
0.0132	-7.61556585E-12	1.00898598E-13	h-NN
0.0001	3.80977648E-10	4.51057048E-14	h-N
0.0011	7.69195129E-12	8.25197184E-15	h
0.0000	-2.79083134E-01	8.34265081E-09	(S)A-K
0.0000	-2.35670741E-02	3.69578458E-09	(S)A-N
0.0000	-1.56515073E-04	5.02119084E-09	(S)a'
0.0002	1.00813330E-06	2.45948525E-10	(S)D-KK
0.0002	1.99300501E-06	3.28330966E-10	(S)D-NK
0.0001	9.99002839E-07	1.12954704E-10	(S)D-NN
0.0001	1.99992091E-06	1.67260616E-10	(S)d-N
0.0001	1.00051655E-06	6.97762553E-11	(S)d'
0.0376	4.96119823E-11	1.86503727E-12	(S)H-KKK
0.0341	-6.35794532E-11	2.17114792E-12	(S)H-NNK
0.0561	1.39632363E-11	7.83890796E-13	(S)H-NNN
0.1620	7.63724397E-12	1.23712196E-12	(S)h-NN
0.1016	-7.19161993E-12	7.30697351E-13	(S)h-N
0.0219	-7.56080512E-12	1.65608517E-13	(S)h'

S-A FITTING FOR A MOLECULE WITH K = -0.99,
A TENDENCY = 10^{-2} IN THE ROTOR PART ONLY

Source	Number	Std. Dev.	Scaled
CALC	241	0.0001 Cm-1	0.0001
All	241	1.6396 MHz	0.0001
Ratio	Cm-1	Std. Dev.	
0.0000	1.31255405E+01	1.83440289E-06	A-K
0.0000	1.05638420E+01	8.16091155E-07	A-N
0.0000	1.63480594E-02	5.47770249E-07	a
0.0005	-9.93537080E-05	4.87735819E-08	D-KK
0.0006	-1.00685247E-04	6.36044868E-08	D-KN
0.0002	-9.98963365E-05	2.20489455E-08	D-NN
0.0001	-1.00000937E-04	6.13701007E-09	d-N
0.0096	-1.06418379E-06	1.02096330E-08	d
0.1410	5.26653128E-09	7.42579600E-10	H-KKK
0.1068	-1.14797558E-08	1.22562726E-09	H-KKN
0.0963	6.29514431E-09	6.06225615E-10	H-KNN
0.2430	-5.85292629E-10	1.42218197E-10	H-NNN
0.2649	3.88544539E-10	1.02921437E-10	h-N
2.8144	6.69463674E-12	1.88413860E-11	h
0.0001	-2.78986747E-01	1.48650960E-05	(S)A-K

0.0002	-2.36032167E-02	4.39462077E-06	(S)A-N
0.7418	-4.16792657E-05	3.09193137E-05	(S)a'
0.1708	-2.56030354E-06	4.37320546E-07	(S)D-NK
0.0306	2.85783858E-06	8.74100021E-08	(S)D-NN
0.2689	-1.17046494E-04	3.14686017E-05	(S)d-K
0.0417	-3.15077761E-05	1.31290261E-06	(S)d-N
0.0386	8.57608228E-08	3.31203107E-09	(S)H-KNK
0.0616	-5.37975360E-08	3.31429755E-09	(S)H-NNK
0.5113	2.92279516E-06	1.49433365E-06	(S)h-KK
0.0391	3.34800093E-05	1.30868759E-06	(S)h-KN

A' FITTING FOR A MOLECULE WITH K = -0.5,
A TENDENCY = 10^{-2}

CALC	241	0.0000 Cm-1	0.0000
All	241	0.0001 MHz	0.0000
	MHz	Std. Dev.	
0.0000	1.31255408E+01	5.49708607E-08	A-K
0.0000	1.05638419E+01	1.57203651E-08	A-N
0.0000	9.34720501E-01	1.10625412E-07	a
0.0000	-1.00020261E-03	3.90656894E-08	D-KK
0.0000	-9.99756148E-04	4.70651687E-08	D-KN
0.0000	-1.00004079E-03	7.86990074E-09	D-NN
0.0001	-1.00057369E-03	1.10606383E-07	d-K
0.0000	-9.99999829E-04	1.14820690E-11	d-N
0.0004	-9.98017991E-06	3.89478204E-09	d
0.0006	1.00258981E-07	5.63583910E-11	H-KKK
0.0004	9.97901481E-08	4.23945312E-11	H-KKN
0.0002	9.99173970E-08	2.34773570E-11	H-KNN
0.0001	1.00032467E-07	7.82249916E-12	H-NNN
0.0002	1.00001441E-07	2.14491716E-11	h-KK
0.0001	9.98562390E-08	8.60936801E-12	h-KN
0.0000	1.00001765E-07	1.90416023E-13	h-NN
0.0107	1.13800030E-09	1.22273558E-11	h-K
0.0040	9.83912574E-10	3.91616358E-12	h-N
0.0002	9.98255438E-10	1.96895882E-13	h
0.0000	-2.79081764E-01	8.72449163E-09	(S)A-K
0.0000	-2.35674613E-02	3.66075619E-09	(S)A-N
0.0000	-9.01266694E-03	5.08539665E-09	(S)a'
0.0001	1.11167277E-05	8.72348286E-10	(S)D-KK
0.0577	2.98990876E-07	1.72436042E-08	(S)D-KN
0.0009	1.83798356E-05	1.69266204E-08	(S)D-NK
0.0000	1.02008842E-05	2.26578231E-10	(S)D-NN
0.0003	1.29059962E-05	3.94877951E-09	(S)d-K
0.0000	1.00957401E-05	2.09741684E-10	(S)d-N
0.8708	1.97183792E-10	1.71699761E-10	(S)H-KKK
0.4664	2.35919703E-09	1.10035621E-09	(S)H-KKN
0.6926	1.25145416E-09	8.66717857E-10	(S)H-KNK
0.0144	-1.74540939E-08	2.51060076E-10	(S)H-KNN
0.0107	1.86526496E-08	1.99896434E-10	(S)H-NNK
0.0028	1.02674788E-09	2.83604212E-12	(S)H-NNN
0.1566	2.28781740E-09	3.58376924E-10	(S)h-KK
0.0067	4.75247949E-09	3.16098758E-11	(S)h-KN
0.0023	1.01523662E-09	2.28548156E-12	(S)h-NN

S' FITTING FOR A MOLECULE WITH K = -0.5,
A TENDENCY = 10^{-2}

All	241	0.0019 MHz	0.0000
Ratio	Cm-1	Std. Dev.	
0.0000	1.31255376E+01	1.02430541E-06	A-K
0.0000	1.05638429E+01	2.93002190E-07	A-N
0.0000	9.34727964E-01	2.06743244E-06	a
0.0007	-1.00282337E-03	7.30251831E-07	D-KK
0.0009	-9.96599519E-04	8.79733513E-07	D-KN
0.0001	-1.00056837E-03	1.47095444E-07	D-NN
0.0021	-1.00800526E-03	2.06732518E-06	d-K
0.0000	-9.99996803E-04	2.67708387E-10	d-N
0.0075	-9.71904409E-06	7.26649947E-08	d
0.0099	1.04018239E-07	1.03420347E-09	H-KKK
0.0079	9.60290362E-08	7.58587557E-10	H-KKN
0.0044	9.95709384E-08	4.33457850E-10	H-KNN
0.0014	1.00363518E-07	1.45336411E-10	H-NNN
0.0017	1.00620892E-07	1.76056341E-10	h-KK
0.0024	9.67875389E-08	2.27673864E-10	h-KN
0.0000	1.00010440E-07	4.15137793E-12	h-NN
0.1709	1.72823385E-09	2.95369365E-10	h-K
0.0884	8.22133718E-10	7.27008035E-11	h-N
0.0042	9.89620020E-10	4.13512124E-12	h
0.0000	-2.79088764E-01	1.70420913E-07	(S)A-K
0.0000	-2.35654397E-02	6.88634923E-08	(S)A-N
0.0000	-8.99978568E-03	6.32334326E-08	(S)a'
0.0032	5.89289266E-06	1.90908655E-08	(S)D-KK
0.0045	4.89261800E-05	2.21253302E-07	(S)D-KN
0.0087	-2.41149360E-05	2.10322180E-07	(S)D-NK
0.0005	9.28505504E-06	4.77843824E-09	(S)D-NN
0.0007	1.00013973E-05	6.93797877E-09	(S)d-N
0.0041	4.61294427E-07	1.90236598E-09	(S)d'
0.1310	2.45429164E-09	3.21419380E-10	(S)H-KKK
0.0445	6.51950268E-08	2.89879343E-09	(S)H-KKN
0.1110	-3.26062532E-08	3.62007350E-09	(S)H-KNK
0.0620	-3.57756996E-08	2.21843578E-09	(S)H-NNK
0.0484	7.36898457E-09	3.56648104E-10	(S)H-NNN
0.0622	9.45443516E-08	5.87779887E-09	(S)h-KN
0.0396	1.04255814E-09	4.12979159E-11	(S)h-NN
0.0574	-3.30784709E-09	1.89752873E-10	(S)h-N
0.9646	-1.62949956E-11	1.57177995E-11	(S)h'

A' FITTING FOR A MOLECULE WITH K = -0.5,
A TENDENCY = 10^{-2} IN THE SPIN-ROTOR PART

Source	Number	Std. Dev.	Scaled
CALC	241	0.0000 Cm-1	0.0000
All	241	0.0019 MHz	0.0000
Ratio	Cm-1	Std. Dev.	
0.0000	1.31255411E+01	8.73763154E-08	A-K
0.0000	1.05638419E+01	2.63535859E-08	A-N
0.0000	9.34720116E-01	1.69272031E-07	a

0.0001	-1.00007755E-03	6.02582656E-08	D-KK
0.0001	-9.99910665E-04	7.24505245E-08	D-KN
0.0000	-1.00001449E-03	1.20919283E-08	D-NN
0.0002	-1.00020389E-03	1.69437512E-07	d-K
0.0000	-9.99999735E-04	1.00960556E-10	d-N
0.0000	-9.99992843E-04	6.24878677E-09	d
0.0014	9.91397966E-08	1.38205392E-10	H-KKK
0.0016	1.01415525E-07	1.62151365E-10	H-KKN
0.0006	9.93954272E-08	6.01273710E-11	H-KNN
0.0001	1.00041214E-07	1.29420136E-11	H-NNN
0.0030	9.79103636E-08	2.89850138E-10	h-KK
0.0008	1.00499567E-07	8.38945186E-11	h-KN
0.0001	1.00004892E-07	1.20987599E-11	h-NN
0.0005	1.00059003E-07	5.17122264E-11	h-K
0.0001	9.99814260E-08	6.43065744E-12	h-N
0.0001	9.99981701E-08	1.20240820E-11	h
0.0000	-2.79082056E-01	1.44070926E-07	(S)A-K
0.0000	-2.35673581E-02	6.23219766E-08	(S)A-N
0.0000	-9.01239836E-03	8.02889328E-08	(S)a'
0.0013	1.11503657E-05	1.47759614E-08	(S)D-KK
0.1442	1.76773312E-06	2.54950715E-07	(S)D-KN
0.0149	1.68939306E-05	2.52561710E-07	(S)D-NK
0.0004	1.02040687E-05	4.08988078E-09	(S)D-NN
0.0046	1.26990361E-05	5.82109614E-08	(S)d-K
0.0004	1.00973761E-05	3.66535790E-09	(S)d-N
0.1158	2.37965454E-08	2.75681028E-09	(S)H-KKK
0.0590	-2.75949623E-07	1.62693655E-08	(S)H-KKN
0.0510	2.46181101E-07	1.25623304E-08	(S)H-KNK
0.0464	5.18599544E-08	2.40797852E-09	(S)H-KNN
0.0446	-4.04763520E-08	1.80362011E-09	(S)H-NNK
0.0602	8.49389622E-10	5.11528320E-11	(S)H-NNN
0.1240	4.74601438E-08	5.88371863E-09	(S)h-KK
0.2868	1.75163549E-09	5.02354292E-10	(S)h-KN
0.0477	8.48801208E-10	4.04509419E-11	(S)h-NN

S'FITTING FOR A MOLECULE WITH K = -0.5,
A TENDENCY = 10^{-2} IN THE SPIN-ROTOR PART

Source	Number	Std. Dev.	Scaled
CALC	241	0.0000 Cm-1	0.0000
All	241	0.0095 MHz	0.0000
Ratio	Cm-1	Std. Dev.	
0.0000	1.31255408E+01	3.22332035E-07	A-K
0.0000	1.05638420E+01	1.01570855E-07	A-N
0.0000	9.34720741E-01	5.88500176E-07	a
0.0002	-1.00026685E-03	2.08860570E-07	D-KK
0.0003	-9.99674354E-04	2.51489685E-07	D-KN
0.0000	-1.00005481E-03	4.20294810E-08	D-NN
0.0006	-1.00075222E-03	5.87103195E-07	d-K
0.0000	-1.00000501E-03	7.07623117E-10	d-N
0.0000	-9.99971656E-04	2.15670462E-08	d
0.0029	1.00002992E-07	2.86770068E-10	H-KKK
0.0031	1.01881005E-07	3.17510580E-10	H-KKN
0.0026	9.77682399E-08	2.53682331E-10	H-KNN

0.0005	1.00369099E-07	5.18102627E-11	H-NNN
0.0031	9.96080906E-08	3.04683109E-10	h-KK
0.0070	1.04926832E-07	7.30659060E-10	h-KN
0.0004	1.00003822E-07	4.41041766E-11	h-NN
0.0015	9.94513635E-08	1.48995127E-10	h-K
0.0003	9.98206939E-08	2.68055361E-11	h-N
0.0004	9.99711264E-08	4.29845781E-11	h
0.0000	-2.79088161E-01	7.44810462E-07	(S)A-K
0.0000	-2.35656901E-02	3.19901494E-07	(S)A-N
0.0000	-8.99974779E-03	3.14901915E-07	(S)a'
0.0087	5.94338680E-06	5.15087097E-08	(S)D-KK
0.0106	3.92860638E-05	4.17054093E-07	(S)D-KN
0.0276	-1.44475634E-05	3.99411412E-07	(S)D-NK
0.0021	9.24422056E-06	1.95158465E-08	(S)D-NN
0.0019	1.01794868E-05	1.94586818E-08	(S)d-N
0.0128	4.87274633E-07	6.24228673E-09	(S)d'
0.0256	4.09101094E-07	1.04834593E-08	(S)H-KKN
0.0266	-4.41786431E-07	1.17436072E-08	(S)H-KNK
0.1106	4.35135191E-08	4.81369683E-09	(S)H-NNK
0.1447	-5.49946224E-09	7.95533003E-10	(S)H-NNN
0.1093	-1.28774368E-07	1.40713819E-08	(S)h-KN
0.0866	3.07737807E-09	2.66431715E-10	(S)h-NN
0.1290	3.30164223E-09	4.25906759E-10	(S)h-N
0.0769	-1.25489994E-09	9.65129517E-11	(S)h'

A' FITTING FOR A MOLECULE WITH K = -0.5,
A TENDENCY = 10^{-2} IN THE ROTOR PART

Source	Number	Std. Dev.	Scaled
CALC	241	0.0000 Cm-1	0.0000
All	241	0.0136 MHz	0.0000
Ratio	Cm-1	Std. Dev.	
0.0000	1.31255334E+01	4.50070712E-07	A-K
0.0000	1.05638427E+01	1.44828345E-07	A-N
0.0000	9.34724867E-01	7.23149114E-07	a
0.0003	-1.00182160E-03	2.60704989E-07	D-KK
0.0003	-9.97806844E-04	3.15171369E-07	D-KN
0.0001	-1.00038114E-03	5.28939282E-08	D-NN
0.0007	-1.00529614E-03	7.21141745E-07	d-K
0.0000	-9.99977306E-04	1.21493355E-09	d-N
0.0026	-9.85060021E-06	2.60606614E-08	d
0.0051	1.00061059E-07	5.05469107E-10	H-KKK
0.0075	9.54546156E-08	7.14911728E-10	H-KKN
0.0020	1.05085303E-07	2.13506758E-10	H-KNN
0.0001	9.93243871E-08	1.20845940E-11	H-NNN
0.0063	9.56561160E-08	6.01518373E-10	h-KK
0.0123	8.10193734E-08	9.99834282E-10	h-KN
0.0001	1.00120268E-07	1.21921610E-11	h-NN
0.0611	1.14409849E-08	6.99077234E-10	h-K
0.0	1.35401888E-09	0.0	h-N
0.0128	8.80011825E-10	1.12631668E-11	h
0.0000	-2.78947397E-01	1.13080477E-06	(S)A-K
0.0000	-2.36079451E-02	4.75061127E-07	(S)A-N
0.0001	-9.28949754E-03	5.53514250E-07	(S)a'

0.0008	1.21048999E-04	1.01025050E-07	(S)D-KK
0.0022	-9.57701569E-04	2.06951824E-06	(S)D-KN
0.0024	8.46168081E-04	2.00432529E-06	(S)D-NK
0.0010	3.00719849E-05	2.88900157E-08	(S)D-NN
0.0010	2.98771165E-04	3.06686619E-07	(S)d-K
0.0013	1.95427513E-05	2.59341791E-08	(S)d-N
0.0620	-6.68434218E-08	4.14145870E-09	(S)H-KKK
0.0462	1.24284596E-07	5.73716623E-09	(S)H-KNK
0.0095	-1.78868325E-06	1.70576905E-08	(S)H-KNN
0.0101	1.73820712E-06	1.76330061E-08	(S)H-NNK
0.0895	4.01951235E-09	3.59546579E-10	(S)H-NNN
0.0588	1.54252669E-07	9.07598756E-09	(S)h-KK
0.0098	3.94210332E-07	3.87218726E-09	(S)h-KN
0.1082	2.74396248E-09	2.96887238E-10	(S)h-NN

S' FITTING FOR A MOLECULE WITH K = -0.5,
A TENDENCY = 10^{-2} IN THE ROTOR PART

CALC	241	0.0000 Cm-1	0.0000
All	241	0.0046 MHz	0.0000
Ratio	Cm-1	Std. Dev.	
0.0000	1.31255336E+01	2.54889331E-06	A-K
0.0000	1.05638442E+01	7.29163325E-07	A-N
0.0000	9.34737566E-01	5.14342931E-06	a
0.0018	-1.00621464E-03	1.81672172E-06	D-KK
0.0022	-9.92513755E-04	2.18867549E-06	D-KN
0.0004	-1.00125139E-03	3.65967467E-07	D-NN
0.0051	-1.01762617E-03	5.14340327E-06	d-K
0.0000	-9.99992116E-04	6.59587130E-10	d-N
0.0193	-9.38153261E-06	1.80699929E-07	d
0.0239	1.08862356E-07	2.60369756E-09	H-KKK
0.0212	9.09576196E-08	1.92806877E-09	H-KKN
0.0107	9.93862056E-08	1.06806530E-09	H-KNN
0.0036	1.00749391E-07	3.62068319E-10	H-NNN
0.0045	1.01302746E-07	4.51177115E-10	h-KK
0.0061	9.20805384E-08	5.58948379E-10	h-KN
0.0001	1.00023422E-07	1.03963645E-11	h-NN
0.2806	2.65790010E-09	7.45745515E-10	h-K
0.2852	6.35026538E-10	1.81117490E-10	h-N
0.0106	9.76743251E-10	1.03540908E-11	h
0.0000	-2.79094502E-01	4.23305875E-07	(S)A-K
0.0000	-2.35637943E-02	1.71127801E-07	(S)A-N
0.0000	-8.99003983E-03	1.57388725E-07	(S)a'
0.0333	1.41737474E-06	4.71367734E-08	(S)D-KK
0.0043	1.25717570E-04	5.39343493E-07	(S)D-KN
0.0053	-9.57714106E-05	5.11885178E-07	(S)D-NK
0.0014	8.60384760E-06	1.18444246E-08	(S)D-NN
0.0009	1.97609196E-05	1.70011489E-08	(S)d-N
0.0004	1.07161431E-05	4.70032871E-09	(S)d'
0.8656	9.22448775E-10	7.98509390E-10	(S)H-KKK
0.0229	3.03354778E-07	6.96048062E-09	(S)H-KKN
0.0386	-2.24961327E-07	8.68627279E-09	(S)H-KNK
0.0615	-8.77752052E-08	5.39871100E-09	(S)H-NNK
0.0541	1.60602526E-08	8.68290232E-10	(S)H-NNN

0.0623	2.30143033E-07	1.43348740E-08	(S)h-KN
0.0506	2.02875167E-09	1.02563383E-10	(S)h-NN
0.0785	-5.88578321E-09	4.62271878E-10	(S)h-N
0.0390	9.84483840E-10	3.83472824E-11	(S)h'

A' FITTING FOR A MOLECULE WITH K = -0.5,
WITHOUT A TENDENCY

Source	Number	Std. Dev.	Scaled
CALC	241	0.0000 Cm-1	0.0005
All	241	0.2191 MHz	0.0005
Ratio	Cm-1	Std. Dev.	
0.0000	1.31254919E+01	1.23476824E-05	A-K
0.0000	1.05638552E+01	3.77790693E-06	A-N
0.0000	9.34824637E-01	2.50991399E-05	a
0.0087	-1.03775073E-03	8.99043869E-06	D-KK
0.0113	-9.54928874E-04	1.07886416E-05	D-KN
0.0018	-1.00753465E-03	1.80394006E-06	D-NN
0.0227	-1.10652334E-03	2.50927380E-05	d-K
0.0000	-9.99983927E-04	1.31733383E-08	d-N
0.0009	-9.96209751E-04	9.21754571E-07	d
0.1857	7.50647850E-08	1.39387059E-08	H-KKK
0.0964	1.89812039E-07	1.83004107E-08	H-KKN
0.4098	2.48712483E-08	1.01934368E-08	H-KNN
0.0169	1.11145699E-07	1.87500203E-09	H-NNN
0.9632	-3.64851261E-08	3.51414251E-08	h-KK
0.0906	1.33556520E-07	1.20956286E-08	h-KN
0.0172	1.06438699E-07	1.83569184E-09	h-NN
0.0606	9.90330098E-08	6.00583363E-09	h-K
0.0097	9.44854982E-08	9.12450089E-10	h-N
0.0193	9.37572069E-08	1.81002947E-09	h
0.0001	-2.79010271E-01	1.68989175E-05	(S)A-K
0.0003	-2.35945583E-02	7.30389932E-06	(S)A-N
0.0010	-9.28441799E-03	9.01391248E-06	(S)a'
0.0132	1.19550709E-04	1.57646837E-06	(S)D-KK
0.0292	-9.17838382E-04	2.68323661E-05	(S)D-KN
0.0323	8.08895018E-04	2.61012511E-05	(S)D-NK
0.0159	2.99006003E-05	4.74835051E-07	(S)D-NN
0.0200	3.04278496E-04	6.08540169E-06	(S)d-K
0.0221	1.92540759E-05	4.24691984E-07	(S)d-N
0.3500	7.13081922E-07	2.49601063E-07	(S)H-KKK
0.0812	-1.93523191E-05	1.57176199E-06	(S)H-KKN
0.0678	1.83629987E-05	1.24432457E-06	(S)H-KNK
0.0602	4.36380585E-06	2.62646678E-07	(S)H-KNN
0.0521	-4.05498157E-06	2.11143070E-07	(S)H-NNK
0.7835	-7.55254953E-09	5.91710933E-09	(S)H-NNN
0.3699	1.51920134E-06	5.61907192E-07	(S)h-KK
0.4122	1.40450371E-07	5.78883423E-08	(S)h-KN
0.3666	-1.29022071E-08	4.72932314E-09	(S)h-NN

S' FITTING FOR A MOLECULE WITH K = -0.5,
WITHOUT A TENDENCY

Source	Number	Std. Dev.	Scaled

CALC	241	0.0000 Cm-1	0.0001
All	241	0.0315 MHz	0.0001
Ratio	Cm-1	Std. Dev.	
0.0000	1.31255385E+01	1.07192170E-06	A-K
0.0000	1.05638428E+01	3.37588667E-07	A-N
0.0000	9.34725564E-01	1.95810392E-06	a
0.0007	-1.00195907E-03	6.94810463E-07	D-KK
0.0008	-9.97629392E-04	8.36637675E-07	D-KN
0.0001	-1.00039740E-03	1.39825646E-07	D-NN
0.0019	-1.00551823E-03	1.95321683E-06	d-K
0.0000	-1.00001665E-03	2.33994318E-09	d-N
0.0001	-9.99795554E-04	7.17436385E-08	d
0.0095	1.01323540E-07	9.58247789E-10	H-KKK
0.0100	1.05439746E-07	1.05507557E-09	H-KKN
0.0091	9.18696844E-08	8.40604094E-10	H-KNN
0.0017	1.01442420E-07	1.72304606E-10	H-NNN
0.0101	1.00354247E-07	1.01151380E-09	h-KK
0.0209	1.14863607E-07	2.40549768E-09	h-KN
0.0015	1.00233014E-07	1.46532791E-10	h-NN
0.0051	9.75500247E-08	4.93328832E-10	h-K
0.0009	9.92960526E-08	8.91640801E-11	h-N
0.0014	9.96843723E-08	1.42951599E-10	h
0.0000	-2.79093295E-01	2.46480294E-06	(S)A-K
0.0000	-2.35643953E-02	1.05864793E-06	(S)A-N
0.0001	-8.98990984E-03	1.04203923E-06	(S)a'
0.1069	1.58863739E-06	1.69788153E-07	(S)D-KK
0.0138	9.65459597E-05	1.32878182E-06	(S)D-KN
0.0191	-6.65122763E-05	1.27187779E-06	(S)D-NK
0.0076	8.47704540E-06	6.45153544E-08	(S)D-NN
0.0032	2.02611758E-05	6.43688872E-08	(S)d-N
0.0019	1.07988365E-05	2.06330155E-08	(S)d'
0.0240	1.34767919E-06	3.24102934E-08	(S)H-KKN
0.0250	-1.46827012E-06	3.67393103E-08	(S)H-KNK
0.1086	1.46144772E-07	1.58654051E-08	(S)H-NNK
0.1219	-2.15051251E-08	2.62247963E-09	(S)H-NNN
0.1112	-4.16818810E-07	4.63613954E-08	(S)h-KN
0.1141	7.71224943E-09	8.80037799E-10	(S)h-NN
0.1054	1.33254921E-08	1.40398760E-09	(S)h-N
0.1518	-2.09545434E-09	3.18170940E-10	(S)h'

A' FITTING FOR A MOLECULE WITH K = -0.9,
A TENDENCY = 10^{-2}

Source	Number	Std. Dev.	Scaled
CALC	241	0.0000 Cm-1	0.0000
All	241	0.0067 MHz	0.0000
Ratio	Cm-1	Std. Dev.	
0.0000	1.31255411E+01	5.63037318E-07	A-K
0.0000	1.05638417E+01	1.32973781E-07	A-N
0.0000	1.68222532E-01	5.11707279E-06	a
0.0003	-9.99690936E-04	3.13590973E-07	D-KK
0.0004	-1.00039113E-03	3.85035098E-07	D-KN
0.0001	-9.99939507E-04	6.53481889E-08	D-NN
0.0051	-9.94905207E-04	5.11611444E-06	d-K

0.0000	-9.99989913E-04	9.15861999E-10	d-N
0.0032	-1.00277959E-05	3.22860968E-08	d
0.0277	9.79744110E-08	2.71594181E-09	H-KKK
0.0196	1.00832282E-07	1.97568795E-09	H-KKN
0.0110	1.01590739E-07	1.12250558E-09	H-KNN
0.0038	9.96197011E-08	3.81182745E-10	H-NNN
0.0095	1.07993218E-07	1.02413044E-09	h-KK
0.0088	8.98037885E-08	7.93277338E-10	h-KN
0.0001	9.99953530E-08	7.84141026E-12	h-NN
0.0	1.00000000E-09	0.0	h-K
0.1605	1.19098667E-09	1.91120878E-10	h-N
0.0036	1.00420487E-09	3.65063838E-12	h
0.0000	-2.79082321E-01	5.58452927E-07	(S)A-K
0.0000	-2.35678575E-02	2.44301206E-07	(S)A-N
0.0004	-1.62796670E-03	6.04323336E-07	(S)a'
0.0491	1.18099086E-05	5.80141114E-07	(S)D-KK
0.4968	-8.85148882E-05	4.39735068E-05	(S)D-KN
0.4077	1.06443704E-04	4.33933292E-05	(S)D-NK
0.0015	1.01706222E-05	1.53836183E-08	(S)D-NN
0.0323	1.65480230E-05	5.34650205E-07	(S)d-K
0.0028	9.91063189E-06	2.78497382E-08	(S)d-N
0.0905	-1.20249755E-06	1.08874057E-07	(S)H-KKN
0.0886	1.22465772E-06	1.08559923E-07	(S)H-KNK
0.2146	-1.05141750E-06	2.25621564E-07	(S)H-KNN
0.2151	1.03515507E-06	2.22689906E-07	(S)H-NNK
0.3152	4.77574440E-10	1.50511245E-10	(S)H-NNN
0.1172	-1.82400118E-07	2.13758709E-08	(S)h-KK
0.1076	1.82478646E-07	1.96418543E-08	(S)h-KN
0.2058	1.10853251E-09	2.28139511E-10	(S)h-NN

S' FITTING FOR A MOLECULE WITH K = -0.9,
A TENDENCY = 10^{-2}

Source	Number	Std. Dev.	Scaled
CALC	241	0.0000 Cm-1	0.0000
All	241	0.0149 MHz	0.0000
Ratio	Cm-1	Std. Dev.	
0.0000	1.31255551E+01	6.80555129E-07	A-K
0.0000	1.05638399E+01	2.38885535E-07	A-N
0.0001	1.68134319E-01	1.02522607E-05	a
0.0006	-9.94305647E-04	6.28610817E-07	D-KK
0.0008	-1.00696531E-03	7.71417505E-07	D-KN
0.0001	-9.98819051E-04	1.30579679E-07	D-NN
0.0113	-9.06709682E-04	1.02482255E-05	d-K
0.0000	-1.00000608E-03	2.50095720E-09	d-N
0.0063	-1.05946540E-05	6.62993003E-08	d
0.0941	5.23592884E-08	4.92509109E-09	H-KKK
0.0242	1.33701587E-07	3.23423281E-09	H-KKN
0.0204	1.20903507E-07	2.46501496E-09	H-KNN
0.0082	9.31489370E-08	7.64288875E-10	H-NNN
0.0060	9.45429008E-08	5.70128705E-10	h-KK
0.0197	1.08612241E-07	2.13929499E-09	h-KN
0.0002	9.99187811E-08	1.77819407E-11	h-NN
0.5462	3.67700012E-09	2.00849715E-09	h-K

0.0865	4.40732683E-09	3.81078687E-10	h-N
0.0089	1.07957526E-09	9.61730030E-12	h
0.0000	-2.79079604E-01	1.32031305E-06	(S)A-K
0.0000	-2.35692193E-02	5.25114713E-07	(S)A-N
0.0004	-1.61084718E-03	6.58316410E-07	(S)a'
0.1568	-3.44457346E-06	5.40062616E-07	(S)D-KK
0.0380	1.02627629E-03	3.90466211E-05	(S)D-KN
0.0388	-9.92454481E-04	3.85390544E-05	(S)D-NK
0.0028	9.87469982E-06	2.74884236E-08	(S)D-NN
0.0074	1.04736077E-05	7.72124298E-08	(S)d-N
0.1100	1.01645337E-07	1.11782410E-08	(S)d'
0.1097	1.50058529E-06	1.64572632E-07	(S)H-KKN
0.1071	-1.54374219E-06	1.65382282E-07	(S)H-KNK
0.0422	4.75307660E-08	2.00384694E-09	(S)H-NNK
0.1647	-3.84975382E-07	6.34034035E-08	(S)h-KN
0.4841	1.05794423E-09	5.12170436E-10	(S)h-NN
0.1847	1.27054850E-09	2.34730255E-10	(S)h-N
0.4122	-3.35301833E-10	1.38220058E-10	(S)h'

A' FITTING FOR A MOLECULE WITH K = -0.9,
A TENDENCY = 10^{-2} IN THE SPIN-ROTOR PART

Source	Number	Std. Dev.	Scaled
CALC	241	0.0000 Cm-1	0.0000
All	241	0.0104 MHz	0.0000
Ratio	Cm-1	Std. Dev.	
0.0000	1.31255409E+01	1.70903374E-07	A-K
0.0000	1.05638420E+01	6.83336074E-08	A-N
0.0000	1.68231065E-01	1.18659430E-06	a
0.0001	-1.00024744E-03	7.80180941E-08	D-KK
0.0001	-9.99732865E-04	9.18347721E-08	D-KN
0.0000	-1.00004443E-03	1.55374458E-08	D-NN
0.0012	-1.00343901E-03	1.18150628E-06	d-K
0.0000	-1.00000145E-03	9.71471469E-10	d-N
0.0000	-9.99968889E-04	8.75260485E-09	d
0.0052	1.01772188E-07	5.29781153E-10	H-KKK
0.0029	9.88696857E-08	2.88017108E-10	H-KKN
0.0035	9.91647848E-08	3.43396304E-10	H-KNN
0.0010	1.00266978E-07	9.62218893E-11	H-NNN
0.0198	1.03027185E-07	2.03752689E-09	h-KK
0.0058	9.97025461E-08	5.77921419E-10	h-KN
0.0009	1.00244040E-07	8.94716513E-11	h-NN
0.0029	9.93855351E-08	2.89139367E-10	h-K
0.0005	9.98416131E-08	4.68056380E-11	h-N
0.0009	9.97541269E-08	8.97085013E-11	h
0.0000	-2.79083725E-01	8.33825209E-07	(S)A-K
0.0000	-2.35671841E-02	3.40526208E-07	(S)A-N
0.0005	-1.62514362E-03	7.38555132E-07	(S)a'
0.0049	1.03627993E-05	5.06245203E-08	(S)D-KK
0.0029	1.96989759E-05	5.67800113E-08	(S)D-NK
0.0019	1.00292993E-05	1.92656689E-08	(S)D-NN
0.0461	1.37341090E-05	6.32794261E-07	(S)d-K
0.0030	1.01072919E-05	2.99100456E-08	(S)d-N
0.1867	4.95851146E-08	9.25948825E-09	(S)H-KKK

0.1773	-4.00172792E-06	7.09488865E-07	(S)H-KKN
0.1772	3.94618234E-06	6.99230290E-07	(S)H-KNK
0.1650	6.58112408E-07	1.08557868E-07	(S)H-KNN
0.1655	-6.47745053E-07	1.07192794E-07	(S)H-NNK
0.2651	8.61473096E-10	2.28365649E-10	(S)H-NNN
0.4111	-8.22462511E-08	3.38085827E-08	(S)h-KK
0.9018	-1.58353148E-08	1.42800391E-08	(S)h-KN
0.3266	1.08625062E-09	3.54735321E-10	(S)h-NN

S' FITTING FOR A MOLECULE WITH K = -0.9,
TENDENCY = 10^{-2} IN THE SPIN-ROTOR PART

Source	Number	Std. Dev.	Scaled
CALC	241	0.0000 Cm-1	0.0001
All	241	0.0581 MHz	0.0001
Ratio	Cm-1	Std. Dev.	
0.0000	1.31255446E+01	9.21266122E-07	A-K
0.0000	1.05638412E+01	3.69475240E-07	A-N
0.0000	1.68201281E-01	5.29631957E-06	a
0.0003	-9.98240947E-04	3.41315055E-07	D-KK
0.0004	-1.00210547E-03	4.12588412E-07	D-KN
0.0001	-9.99668555E-04	6.94658250E-08	D-NN
0.0055	-9.73929552E-04	5.31469385E-06	d-K
0.0000	-9.99994986E-04	5.19178510E-09	d-N
0.0000	-1.00019117E-03	4.01139262E-08	d
0.0252	8.85208209E-08	2.22731203E-09	H-KKK
0.0099	1.05750716E-07	1.04875862E-09	H-KKN
0.0152	1.08557753E-07	1.64706103E-09	H-KNN
0.0044	9.79334742E-08	4.33525294E-10	H-NNN
0.1226	3.97891815E-08	4.87900658E-09	h-KK
0.0260	1.06899227E-07	2.78356854E-09	h-KN
0.0041	9.81555294E-08	4.03114159E-10	h-NN
0.0133	1.06839302E-07	1.41714828E-09	h-K
0.0022	1.01035457E-07	2.18263913E-10	h-N
0.0040	1.01882710E-07	4.02867851E-10	h
0.0000	-2.79103047E-01	4.59355434E-06	(S)A-K
0.0001	-2.35668646E-02	1.90028338E-06	(S)A-N
0.0011	-1.61021076E-03	1.71329043E-06	(S)a'
0.0260	1.11586268E-05	2.90355449E-07	(S)D-KK
0.0539	-2.05938441E-04	1.10911007E-05	(S)D-KN
0.0489	2.25172371E-04	1.10159627E-05	(S)D-NK
0.0106	9.86645602E-06	1.04364718E-07	(S)D-NN
0.0127	1.01690036E-05	1.29354649E-07	(S)d-N
0.2135	1.77680579E-07	3.79323305E-08	(S)d'
0.0525	-2.38351474E-07	1.25153718E-08	(S)H-KKK
0.0397	1.38541812E-05	5.50310135E-07	(S)H-KKN
0.0399	-1.35767047E-05	5.42371139E-07	(S)H-KNK
0.1927	-3.76504806E-08	7.25567575E-09	(S)H-NNK
0.4080	3.08919226E-09	1.26048443E-09	(S)H-NNN
1.1815	6.41415612E-08	7.57857485E-08	(S)h-KN
0.6190	-1.05823205E-09	6.55073453E-10	(S)h-N

A' FITTING FOR A MOLECULE WITH K = -0.9,

A TENDENCY = 10^{-2} IN THE ROTOR PART

Source	Number	Std. Dev.	Scaled
CALC	241	0.0000 Cm-1	0.0017
All	241	0.8022 MHz	0.0019
Ratio	Cm-1	Std. Dev.	
0.0000	1.31257353E+01	1.33405564E-05	A-K
0.0000	1.05637949E+01	5.44283913E-06	A-N
0.0002	1.66156074E-01	3.94788813E-05	a
0.0025	-8.69342428E-04	2.18364611E-06	D-KK
0.0022	-1.15721389E-03	2.57650692E-06	D-KN
0.0005	-9.73965665E-04	4.80095526E-07	D-NN
0.0373	1.06765688E-03	3.98159328E-05	d-K
0.0001	-9.98993007E-04	1.26579589E-07	d-N
0.0138	-2.40899921E-05	3.31578944E-07	d
0.0	2.13621169E-07	0.0	H-KKK
0.0152	-8.41066194E-07	1.28006800E-08	H-KKN
0.0134	1.08395072E-06	1.45509046E-08	H-KNN
0.0510	-5.47222754E-08	2.79070394E-09	H-NNN
0.1873	1.52315435E-06	2.85295485E-07	h-KK
0.1212	-9.11275236E-07	1.10434394E-07	h-KN
0.0023	9.86755749E-08	2.23814989E-10	h-NN
0.1110	3.73370787E-07	4.14556928E-08	h-K
0.0179	7.77645229E-08	1.39119975E-09	h-N
0.0233	2.44711737E-09	5.71112962E-11	h
0.0002	-2.78882076E-01	6.90625305E-05	(S)A-K
0.0012	-2.36651897E-02	2.94618699E-05	(S)A-N
0.0333	-1.94696353E-03	6.48949451E-05	(S)a'
0.6456	1.96627364E-05	1.26950547E-05	(S)D-KK
0.2829	3.10571690E-03	8.78674523E-04	(S)D-KN
0.2791	-3.10979160E-03	8.67969437E-04	(S)D-NK
0.0763	2.40591880E-05	1.83469824E-06	(S)D-NN
0.1693	3.81484486E-04	6.45891302E-05	(S)d-K
0.5889	4.98053734E-06	2.93281884E-06	(S)d-N
0.2078	-1.36839129E-06	2.84289383E-07	(S)H-KKK
0.1265	6.29926347E-05	7.96610032E-06	(S)H-KKN
0.1270	-6.07411639E-05	7.71126989E-06	(S)H-KNK
0.0961	-4.55995898E-05	4.38293662E-06	(S)H-KNN
0.0959	4.47719021E-05	4.29146565E-06	(S)H-NNK
0.9165	-2.17326193E-08	1.99182146E-08	(S)H-NNN
0.1575	-2.05180376E-05	3.23164412E-06	(S)h-KK
0.1751	1.57368588E-05	2.75484050E-06	(S)h-KN

S' FITTING FOR A MOLECULE WITH K = -0.9,
A TENDENCY = 10^{-2} IN THE ROTOR PART

Source	Number	Std. Dev.	Scaled
CALC	241	0.0000 Cm-1	0.0001
All	241	0.0414 MHz	0.0001
Ratio	Cm-1	Std. Dev.	
0.0000	1.31255364E+01	2.91584965E-06	A-K
0.0000	1.05638397E+01	8.88083190E-07	A-N
0.0002	1.68142311E-01	3.44832092E-05	a
0.0021	-9.94802472E-04	2.11301913E-06	D-KK
0.0026	-1.00634440E-03	2.59218596E-06	D-KN

0.0004	-9.98913954E-04	4.40125762E-07	D-NN
0.0377	-9.14962231E-04	3.44769112E-05	d-K
0.0000	-9.99985572E-04	4.09332973E-09	d-N
0.0205	-1.06318412E-05	2.18203681E-07	d
0.2930	5.71916556E-08	1.67586707E-08	H-KKK
0.0859	1.29161892E-07	1.10923863E-08	H-KKN
0.0687	1.20006318E-07	8.23932862E-09	H-KNN
0.0274	9.36570574E-08	2.56918265E-09	H-NNN
0.0184	9.61481290E-08	1.76955122E-09	h-KK
0.0259	9.83826179E-08	2.54497736E-09	h-KN
0.0005	9.98639874E-08	4.99524697E-11	h-NN
0.1559	2.44283101E-08	3.80809675E-09	h-K
0.3071	4.18873343E-09	1.28615625E-09	h-N
0.0251	1.11586182E-09	2.79625328E-11	h
0.0000	-2.79085510E-01	3.50313269E-06	(S)A-K
0.0001	-2.35671124E-02	1.45855669E-06	(S)A-N
0.0011	-1.60094857E-03	1.82048530E-06	(S)a'
0.0140	3.38841724E-05	4.75193602E-07	(S)D-KK
0.0114	-1.92058642E-03	2.18955870E-05	(S)D-KN
0.0112	1.91695731E-03	2.14735621E-05	(S)D-NK
0.0091	9.80449961E-06	8.89950253E-08	(S)D-NN
0.0060	1.98860903E-05	1.19905088E-07	(S)d-N
0.0033	1.01321969E-05	3.34803567E-08	(S)d'
0.6521	8.60454377E-09	5.61136063E-09	(S)H-KKK
0.1075	-8.46239749E-08	9.09625824E-09	(S)H-KNK
0.0659	8.06309670E-08	5.31557325E-09	(S)H-NNK
0.4924	1.91756991E-09	9.44179202E-10	(S)H-NNN
0.4442	3.18621742E-09	1.41538834E-09	(S)h-NN
0.4830	1.01190151E-09	4.88721364E-10	(S)h-N
0.2998	-8.05549866E-10	2.41504728E-10	(S)h'

S' FITTING FOR A MOLECULE WITH K = -0.9,
WITHOUT A TENDENCY

Source	Number	Std. Dev.	Scaled
CALC	241	0.0000 Cm-1	0.0009
All	241	0.4211 MHz	0.0010
Ratio	Cm-1	Std. Dev.	
0.0000	1.31255673E+01	5.96175785E-06	A-K
0.0000	1.05638381E+01	2.52197241E-06	A-N
0.0001	1.68060711E-01	2.26911077E-05	a
0.0015	-9.89205311E-04	1.47978510E-06	D-KK
0.0017	-1.01328603E-03	1.76096917E-06	D-KN
0.0003	-9.97918725E-04	2.97037512E-07	D-NN
0.0270	-8.38796735E-04	2.26280952E-05	d-K
0.0000	-9.99999737E-04	3.63101079E-08	d-N
0.0002	-1.00122192E-03	1.76317635E-07	d
0.2108	3.43544851E-08	7.24163016E-09	H-KKK
0.0237	1.27879595E-07	3.02644307E-09	H-KKN
0.0523	1.55640649E-07	8.14431942E-09	H-KNN
0.0216	8.71733678E-08	1.87899894E-09	H-NNN
0.1114	-3.17925156E-07	3.54327117E-08	h-KK
0.1322	2.29615748E-07	3.03548462E-08	h-KN
0.0198	8.78797446E-08	1.74219137E-09	h-NN

0.0472	1.46569549E-07	6.91416244E-09	h-K
0.0085	1.06316255E-07	9.06076499E-10	h-N
0.0157	1.12221555E-07	1.75667848E-09	h
0.0001	-2.79211467E-01	3.36036602E-05	(S)A-K
0.0006	-2.35651066E-02	1.39055706E-05	(S)A-N
0.0090	-1.56637990E-03	1.40428773E-05	(S)a'
0.5057	4.34617920E-06	2.19769351E-06	(S)D-KK
0.1396	-4.27860887E-04	5.97160830E-05	(S)D-KN
0.1289	4.56670972E-04	5.88812843E-05	(S)D-NK
0.0923	8.91423278E-06	8.22941900E-07	(S)D-NN
0.0461	2.21285826E-05	1.02028042E-06	(S)d-N
0.0264	1.05032395E-05	2.77603278E-07	(S)d'
0.0920	-8.64792565E-07	7.95937517E-08	(S)H-KKK
0.0543	3.44095175E-05	1.86739718E-06	(S)H-KKN
0.0548	-3.33217353E-05	1.82684581E-06	(S)H-KNK
0.1936	-2.50608243E-07	4.85251991E-08	(S)H-NNK
0.7121	1.27575812E-08	9.08493376E-09	(S)H-NNN
0.5257	-1.19947624E-06	6.30605586E-07	(S)h-KN
0.6146	-7.17676936E-09	4.41099137E-09	(S)h'

A' FITTING FOR A MOLECULE WITH K = -0.5,
A TENDENCY = 10^{-2}
WITHOUT USING THE ROTOR PART

Source	Number	Std. Dev.	Scaled
CALC	241	0.0000 Cm-1	0.0000
All	241	0.0022 MHz	0.0000
Ratio	Cm-1	Std. Dev.	
0.0	1.31255412E+01	0.0	A-K
0.0	1.05638418E+01	0.0	A-N
0.0	9.34719932E-01	0.0	a
0.0	-1.00000000E-03	0.0	D-KK
0.0	-1.00000000E-03	0.0	D-KN
0.0	-1.00000000E-03	0.0	D-NN
0.0	-1.00000000E-03	0.0	d-K
0.0	-1.00000000E-03	0.0	d-N
0.0	-1.00000000E-05	0.0	d
0.0	1.00000000E-07	0.0	H-KKK
0.0	1.00000000E-07	0.0	H-KKN
0.0	1.00000000E-07	0.0	H-KNN
0.0	1.00000000E-07	0.0	H-NNN
0.0	1.00000000E-07	0.0	h-KK
0.0	1.00000000E-07	0.0	h-KN
0.0	1.00000000E-07	0.0	h-NN
0.0	1.00000000E-09	0.0	h-K
0.0	1.00000000E-09	0.0	h-N
0.0	1.00000000E-09	0.0	h
0.0000	-2.79081903E-01	3.14319893E-08	(S)A-K
0.0000	-2.35675210E-02	1.34996018E-08	(S)A-N
0.0000	-9.01263173E-03	1.61259278E-08	(S)a'
0.0004	1.11110260E-05	4.69755082E-09	(S)D-KK
0.2725	9.83154847E-07	2.67939835E-07	(S)D-KN
0.0149	1.76851443E-05	2.63407693E-07	(S)D-NK
0.0001	1.02020496E-05	5.91251592E-10	(S)D-NN

0.0005	1.28368603E-05	6.87957104E-09	(S)d-K
0.0000	1.00956356E-05	4.28393438E-10	(S)d-N
0.0877	1.84511845E-09	1.61786776E-10	(S)H-KKK
0.5809	-8.19631830E-09	4.76087656E-09	(S)H-KKN
0.4786	9.58695436E-09	4.58834924E-09	(S)H-KNK
0.1692	-1.97800117E-08	3.34637428E-09	(S)H-KNN
0.1517	2.15745624E-08	3.27298354E-09	(S)H-NNK
0.0050	1.02733455E-09	5.12044935E-12	(S)H-NNN
0.0485	6.26905653E-09	3.04144349E-10	(S)h-KK
0.0138	5.00190029E-09	6.89424876E-11	(S)h-KN
0.0028	1.01577937E-09	2.86147741E-12	(S)h-NN

S' FITTING FOR A MOLECULE WITH K = -0.5,
A TENDENCY = 10^{-2}
WITHOUT USING THE ROTOR PART

Source	Number	Std. Dev.	Scaled
CALC	241	0.0000 Cm-1	0.0000
All	241	0.0068 MHz	0.0000
Ratio	Cm-1	Std. Dev.	
0.0	1.31255412E+01	0.0	A-K
0.0	1.05638418E+01	0.0	A-N
0.0	9.34719932E-01	0.0	a
0.0	-1.00000000E-03	0.0	D-KK
0.0	-1.00000000E-03	0.0	D-KN
0.0	-1.00000000E-03	0.0	D-NN
0.0	-1.00000000E-03	0.0	d-K
0.0	-1.00000000E-03	0.0	d-N
0.0	-1.00000000E-05	0.0	d
0.0	1.00000000E-07	0.0	H-KKK
0.0	1.00000000E-07	0.0	H-KKN
0.0	1.00000000E-07	0.0	H-KNN
0.0	1.00000000E-07	0.0	H-NNN
0.0	1.00000000E-07	0.0	h-KK
0.0	1.00000000E-07	0.0	h-KN
0.0	1.00000000E-07	0.0	h-NN
0.0	1.00000000E-09	0.0	h-K
0.0	1.00000000E-09	0.0	h-N
0.0	1.00000000E-09	0.0	h
0.0000	-2.79086667E-01	8.77778655E-08	(S)A-K
0.0000	-2.35656215E-02	3.93402712E-08	(S)A-N
0.0000	-8.99962374E-03	4.23211533E-08	(S)a'
0.0010	5.91992140E-06	6.14488857E-09	(S)D-KK
0.0091	5.09089157E-05	4.64031177E-07	(S)D-KN
0.0176	-2.60364363E-05	4.58238468E-07	(S)D-NK
0.0001	9.27891327E-06	1.08089078E-09	(S)D-NN
0.0001	1.01028581E-05	1.24006906E-09	(S)d-N
0.0014	4.58584128E-07	6.34131398E-10	(S)d'
0.0253	4.45127822E-09	1.12774546E-10	(S)H-KKK
0.1432	6.29449198E-08	9.01646632E-09	(S)H-KKN
0.1409	-6.31518002E-08	8.89841778E-09	(S)H-KNK
0.0042	1.64100457E-09	6.81608968E-12	(S)H-NNN
0.0084	1.00498396E-09	8.41074991E-12	(S)h-NN
0.0213	-2.84862033E-10	6.06169606E-12	(S)h-N

0.1451	1.01752831E-11	1.47656972E-12	(S)h'

A' FITTING FOR A MOLECULE WITH K = -0.5,
A TENDENCY = 10^{-2} IN THE SPIN-ROTOR PART
WITHOUT USING THE ROTOR PART

Source	Number	Std. Dev.	Scaled
CALC	241	0.0000 Cm-1	0.0001
All	241	0.0282 MHz	0.0001
Ratio	Cm-1	Std. Dev.	
0.0	1.31255412E+01	0.0	A-K
0.0	1.05638418E+01	0.0	A-N
0.0	9.34719932E-01	0.0	a
0.0	-1.00000000E-03	0.0	D-KK
0.0	-1.00000000E-03	0.0	D-KN
0.0	-1.00000000E-03	0.0	D-NN
0.0	-1.00000000E-03	0.0	d-K
0.0	-1.00000000E-03	0.0	d-N
0.0	-1.00000000E-03	0.0	d
0.0	1.00000000E-07	0.0	H-KKK
0.0	1.00000000E-07	0.0	H-KKN
0.0	1.00000000E-07	0.0	H-KNN
0.0	1.00000000E-07	0.0	H-NNN
0.0	1.00000000E-07	0.0	h-KK
0.0	1.00000000E-07	0.0	h-KN
0.0	1.00000000E-07	0.0	h-NN
0.0	1.00000000E-07	0.0	h-K
0.0	1.00000000E-07	0.0	h-N
0.0	1.00000000E-07	0.0	h
0.0000	-2.79079426E-01	3.94997410E-07	(S)A-K
0.0000	-2.35680507E-02	1.70407170E-07	(S)A-N
0.0000	-9.01222230E-03	1.88560025E-07	(S)a'
0.0026	1.10560064E-05	2.86046394E-08	(S)D-KK
0.0018	1.86900413E-05	3.41377872E-08	(S)D-KN
0.0007	1.02384145E-05	6.99837268E-09	(S)D-NN
0.0067	1.19921133E-05	8.00735081E-08	(S)d-K
0.0005	1.01225237E-05	5.29489688E-09	(S)d-N
0.0532	5.68847212E-08	3.02908780E-09	(S)H-KKK
0.1512	-3.32187029E-07	5.02306417E-08	(S)H-KKN
0.1805	2.57743068E-07	4.65236710E-08	(S)H-KNK
0.1071	-1.46249754E-07	1.56612740E-08	(S)H-KNN
0.0861	1.69505180E-07	1.45982363E-08	(S)H-NNK
0.1055	5.80993777E-10	6.13211490E-11	(S)H-NNN
0.0468	1.30591476E-07	6.11764193E-09	(S)h-KK
0.9610	8.49349283E-10	8.16207496E-10	(S)h-KN
0.0478	7.47518576E-10	3.57075656E-11	(S)h-NN

S' FITTING FOR A MOLECULE WITH K = -0.5,
A TENDENCY = 10^{-2} IN THE SPIN-ROTOR PART
WITHOUT USING THE ROTOR PART

Source	Number	Std. Dev.	Scaled
CALC	241	0.0000 Cm-1	0.0000
All	241	0.0157 MHz	0.0000

Ratio	Cm-1	Std. Dev.	
0.0	1.31255412E+01	0.0	A-K
0.0	1.05638418E+01	0.0	A-N
0.0	9.34719932E-01	0.0	a
0.0	-1.00000000E-03	0.0	D-KK
0.0	-1.00000000E-03	0.0	D-KN
0.0	-1.00000000E-03	0.0	D-NN
0.0	-1.00000000E-03	0.0	d-K
0.0	-1.00000000E-03	0.0	d-N
0.0	-1.00000000E-03	0.0	d
0.0	1.00000000E-07	0.0	H-KKK
0.0	1.00000000E-07	0.0	H-KKN
0.0	1.00000000E-07	0.0	H-KNN
0.0	1.00000000E-07	0.0	H-NNN
0.0	1.00000000E-07	0.0	h-KK
0.0	1.00000000E-07	0.0	h-KN
0.0	1.00000000E-07	0.0	h-NN
0.0	1.00000000E-07	0.0	h-K
0.0	1.00000000E-07	0.0	h-N
0.0	1.00000000E-07	0.0	h
0.0000	-2.79087377E-01	2.20611088E-07	(S)A-K
0.0000	-2.35655231E-02	9.55514495E-08	(S)A-N
0.0000	-8.99957780E-03	9.73575984E-08	(S)a'
0.0019	6.05544872E-06	1.12168029E-08	(S)D-KK
0.0122	3.86330029E-05	4.73235647E-07	(S)D-KN
0.0337	-1.38839399E-05	4.67936239E-07	(S)D-NK
0.0003	9.26651757E-06	3.07622531E-09	(S)D-NN
0.0003	1.00979792E-05	2.87566296E-09	(S)d-N
0.0030	4.64526893E-07	1.38370602E-09	(S)d'
0.3688	-5.64147164E-10	2.08031953E-10	(S)H-KKK
0.0428	3.43392160E-07	1.46803232E-08	(S)H-KKN
0.0428	-3.38252972E-07	1.44680214E-08	(S)H-KNK
0.0100	1.57366022E-09	1.57993144E-11	(S)H-NNN
0.0447	-6.92811345E-09	3.09696537E-10	(S)h-KN
0.0116	1.83642699E-09	2.13902212E-11	(S)h-NN
0.0637	-2.53276693E-10	1.61411181E-11	(S)h-N
0.0058	-7.50092813E-10	4.33499500E-12	(S)h'

A' FITTING FOR A MOLECULE WITH K = -0.5,
A TENDENCY = 10^{-2} IN THE ROTOR PART
WITHOUT USING THE ROTOR PART

Source	Number	Std. Dev.	Scaled
CALC	241	0.0000 Cm-1	0.0005
All	241	0.2144 MHz	0.0005
Ratio	Cm-1	Std. Dev.	
0.0	1.31255412E+01	0.0	A-K
0.0	1.05638418E+01	0.0	A-N
0.0	9.34719932E-01	0.0	a
0.0	-1.00000000E-03	0.0	D-KK
0.0	-1.00000000E-03	0.0	D-KN
0.0	-1.00000000E-03	0.0	D-NN
0.0	-1.00000000E-03	0.0	d-K
0.0	-1.00000000E-03	0.0	d-N

0.0	-1.00000000E-05	0.0	d
0.0	1.00000000E-07	0.0	H-KKK
0.0	1.00000000E-07	0.0	H-KKN
0.0	1.00000000E-07	0.0	H-KNN
0.0	1.00000000E-07	0.0	H-NNN
0.0	1.00000000E-07	0.0	h-KK
0.0	1.00000000E-07	0.0	h-KN
0.0	1.00000000E-07	0.0	h-NN
0.0	1.00000000E-09	0.0	h-K
0.0	1.00000000E-09	0.0	h-N
0.0	1.00000000E-09	0.0	h
0.0000	-2.78957286E-01	3.15527170E-06	(S)A-K
0.0001	-2.36101201E-02	1.33461478E-06	(S)A-N
0.0002	-9.28772635E-03	1.56450784E-06	(S)a'
0.0029	1.22759672E-04	3.57325024E-07	(S)D-KK
0.0232	-9.35989479E-04	2.17211696E-05	(S)D-KN
0.0261	8.21032638E-04	2.14341920E-05	(S)D-NK
0.0019	3.02069524E-05	5.77984417E-08	(S)D-NN
0.0022	2.94590431E-04	6.39983178E-07	(S)d-K
0.0021	1.95467159E-05	4.17116197E-08	(S)d-N
0.1751	6.52447619E-08	1.14226637E-08	(S)H-KKK
0.2231	-7.41355520E-08	1.65397396E-08	(S)H-KNK
0.0849	-2.13049064E-06	1.80805204E-07	(S)H-KNN
0.0829	2.15226453E-06	1.78483741E-07	(S)H-NNK
0.1273	3.86481615E-09	4.92053111E-10	(S)H-NNN
0.0534	5.07593121E-07	2.70913020E-08	(S)h-KK
0.0151	4.06829245E-07	6.14183135E-09	(S)h-KN
0.0978	2.85805927E-09	2.79639147E-10	(S)h-NN

S' FITTING FOR A MOLECULE WITH K = -0.5,
A TENDENCY = 10^{-2} IN THE ROTOR PART
WITHOUT USING THE ROTOR PART

Source	Number	Std. Dev.	Scaled
CALC	241	0.0000 Cm-1	0.0000
All	241	0.0205 MHz	0.0000
Ratio	Cm-1	Std. Dev.	
0.0	1.31255412E+01	0.0	A-K
0.0	1.05638418E+01	0.0	A-N
0.0	9.34719932E-01	0.0	a
0.0	-1.00000000E-03	0.0	D-KK
0.0	-1.00000000E-03	0.0	D-KN
0.0	-1.00000000E-03	0.0	D-NN
0.0	-1.00000000E-03	0.0	d-K
0.0	-1.00000000E-03	0.0	d-N
0.0	-1.00000000E-05	0.0	d
0.0	1.00000000E-07	0.0	H-KKK
0.0	1.00000000E-07	0.0	H-KKN
0.0	1.00000000E-07	0.0	H-KNN
0.0	1.00000000E-07	0.0	H-NNN
0.0	1.00000000E-07	0.0	h-KK
0.0	1.00000000E-07	0.0	h-KN
0.0	1.00000000E-07	0.0	h-NN
0.0	1.00000000E-09	0.0	h-K

0.0	1.00000000E-09	0.0	h-N
0.0	1.00000000E-09	0.0	h
0.0000	-2.79088875E-01	2.87832988E-07	(S)A-K
0.0000	-2.35640755E-02	1.24698966E-07	(S)A-N
0.0000	-8.98999765E-03	1.28097835E-07	(S)a'
0.0146	1.46637155E-06	2.14002081E-08	(S)D-KK
0.0102	1.31169436E-04	1.33634105E-06	(S)D-KN
0.0131	-1.01016104E-04	1.31842779E-06	(S)D-NK
0.0005	8.58458669E-06	3.97403831E-09	(S)D-NN
0.0002	1.99984748E-05	3.76319665E-09	(S)d-N
0.0002	1.07128064E-05	1.89885320E-09	(S)d'
0.0588	5.65964252E-09	3.32535011E-10	(S)H-KKK
0.0894	2.88705444E-07	2.57961930E-08	(S)H-KKN
0.0876	-2.90559100E-07	2.54472975E-08	(S)H-KNK
0.0104	1.99714365E-09	2.07868810E-11	(S)H-NNN
0.1259	-3.01217970E-09	3.79246376E-10	(S)h-KN
0.0133	1.98860863E-09	2.64640963E-11	(S)h-NN
0.0139	1.54328437E-09	2.14705407E-11	(S)h-N
0.0043	1.03107887E-09	4.45273025E-12	(S)h'

A' FITTING FOR A MOLECULE WITH K = -0.5,
WITHOUT A TENDENCY
WITHOUT USING THE ROTOR PART

Source	Number	Std. Dev.	Scaled
CALC	241	0.0001 Cm-1	0.0081
All	241	3.5534 MHz	0.0084
Ratio	Cm-1	Std. Dev.	
0.0	1.31255412E+01	0.0	A-K
0.0	1.05638418E+01	0.0	A-N
0.0	9.34719932E-01	0.0	a
0.0	-1.00000000E-03	0.0	D-KK
0.0	-1.00000000E-03	0.0	D-KN
0.0	-1.00000000E-03	0.0	D-NN
0.0	-1.00000000E-03	0.0	d-K
0.0	-1.00000000E-03	0.0	d-N
0.0	-1.00000000E-03	0.0	d
0.0	1.00000000E-07	0.0	H-KKK
0.0	1.00000000E-07	0.0	H-KKN
0.0	1.00000000E-07	0.0	H-KNN
0.0	1.00000000E-07	0.0	H-NNN
0.0	1.00000000E-07	0.0	h-KK
0.0	1.00000000E-07	0.0	h-KN
0.0	1.00000000E-07	0.0	h-NN
0.0	1.00000000E-07	0.0	h-K
0.0	1.00000000E-07	0.0	h-N
0.0	1.00000000E-07	0.0	h
0.0002	-2.78669888E-01	5.11299202E-05	(S)A-K
0.0009	-2.36090348E-02	2.20050527E-05	(S)A-N
0.0026	-9.24171959E-03	2.42551108E-05	(S)a'
0.0334	1.31724062E-04	4.40272680E-06	(S)D-KK
0.2450	5.69694204E-04	1.39569777E-04	(S)D-KN
0.1973	-6.99006951E-04	1.37932832E-04	(S)D-NK
0.0280	3.19589935E-05	8.96153887E-07	(S)D-NN

0.0448	2.28667960E-04	1.02477189E-05	(S)d-K
0.0311	2.12507848E-05	6.61897410E-07	(S)d-N
0.0484	4.15094501E-06	2.00849186E-07	(S)H-KKK
0.0490	-5.85223239E-06	2.86918743E-07	(S)H-KNK
0.0646	-2.21726722E-05	1.43190072E-06	(S)H-KNN
0.0603	2.39857956E-05	1.44606863E-06	(S)H-NNK
0.3145	-2.42961202E-08	7.64233481E-09	(S)H-NNN
0.0469	1.04467224E-05	4.89779708E-07	(S)h-KK
0.8384	1.16302027E-07	9.75102559E-08	(S)h-KN
0.2214	-2.03224123E-08	4.49932000E-09	(S)h-NN

S' FITTING FOR A MOLECULE WITH K = -0.5,
WITHOUT A TENDENCY
WITHOUT USING THE ROTOR PART

Source	Number	Std. Dev.	Scaled
CALC	241	0.0000 Cm-1	0.0001
All	241	0.0505 MHz	0.0001
Ratio	Cm-1	Std. Dev.	
0.0	1.31255412E+01	0.0	A-K
0.0	1.05638418E+01	0.0	A-N
0.0	9.34719932E-01	0.0	a
0.0	-1.00000000E-03	0.0	D-KK
0.0	-1.00000000E-03	0.0	D-KN
0.0	-1.00000000E-03	0.0	D-NN
0.0	-1.00000000E-03	0.0	d-K
0.0	-1.00000000E-03	0.0	d-N
0.0	-1.00000000E-03	0.0	d
0.0	1.00000000E-07	0.0	H-KKK
0.0	1.00000000E-07	0.0	H-KKN
0.0	1.00000000E-07	0.0	H-KNN
0.0	1.00000000E-07	0.0	H-NNN
0.0	1.00000000E-07	0.0	h-KK
0.0	1.00000000E-07	0.0	h-KN
0.0	1.00000000E-07	0.0	h-NN
0.0	1.00000000E-07	0.0	h-K
0.0	1.00000000E-07	0.0	h-N
0.0	1.00000000E-07	0.0	h
0.0000	-2.79090721E-01	7.06672154E-07	(S)A-K
0.0000	-2.35638080E-02	3.06632069E-07	(S)A-N
0.0000	-8.98985231E-03	3.12371185E-07	(S)a'
0.0187	1.89696774E-06	3.54334619E-08	(S)D-KK
0.0153	9.38182583E-05	1.43090579E-06	(S)D-KN
0.0221	-6.40752121E-05	1.41419115E-06	(S)D-NK
0.0012	8.55059143E-06	9.86966983E-09	(S)D-NN
0.0005	1.99830741E-05	9.22725510E-09	(S)d-N
0.0004	1.07283145E-05	4.43057655E-09	(S)d'
0.0763	-8.53934057E-09	6.51342373E-10	(S)H-KKK
0.0383	1.14886236E-06	4.39749436E-08	(S)H-KKN
0.0381	-1.13542345E-06	4.33038909E-08	(S)H-KNK
0.0269	1.88706408E-09	5.08413201E-11	(S)H-NNN
0.0559	-1.78074725E-08	9.94714349E-10	(S)h-KN
0.0184	3.73142818E-09	6.86144469E-11	(S)h-NN
0.0321	1.61366293E-09	5.17836595E-11	(S)h-N

0.0291	-4.76339271E-10	1.38506017E-11	(S)h'

A' FITTING FOR A MOLECULE WITH K = -0.9,
A TENDENCY = 10^{-2}
WITHOUT USING THE ROTOR PART

Source	Number	Std. Dev.	Scaled
CALC	241	0.0000 Cm-1	0.0001
All	241	0.0635 MHz	0.0001
Ratio	Cm-1	Std. Dev.	
0.0	1.31255412E+01	0.0	A-K
0.0	1.05638418E+01	0.0	A-N
0.0	1.68227617E-01	0.0	a
0.0	-1.00000000E-03	0.0	D-KK
0.0	-1.00000000E-03	0.0	D-KN
0.0	-1.00000000E-03	0.0	D-NN
0.0	-1.00000000E-03	0.0	d-K
0.0	-1.00000000E-03	0.0	d-N
0.0	-1.00000000E-05	0.0	d
0.0	1.00000000E-07	0.0	H-KKK
0.0	1.00000000E-07	0.0	H-KKN
0.0	1.00000000E-07	0.0	H-KNN
0.0	1.00000000E-07	0.0	H-NNN
0.0	1.00000000E-07	0.0	h-KK
0.0	1.00000000E-07	0.0	h-KN
0.0	1.00000000E-09	0.0	h-NN
0.0	1.00000000E-09	0.0	h-K
0.0	1.00000000E-09	0.0	h-N
0.0000	-2.79080369E-01	2.20588120E-06	h
0.0000	-2.35705437E-02	3.42292810E-07	(S)A-K
0.0004	-1.62496211E-03	6.71934628E-07	(S)A-N
0.0468	1.28073116E-05	5.98843037E-07	(S)a'
0.2596	-1.76173460E-04	4.57259717E-05	(S)D-KK
0.2341	1.92614721E-04	4.50974059E-05	(S)D-KN
0.0011	1.03010090E-05	1.13084216E-08	(S)D-NK
0.0370	1.38165501E-05	5.10599356E-07	(S)D-NN
0.0016	9.73286659E-06	1.56427062E-08	(S)d-K
0.1046	5.77006816E-08	6.03261987E-09	(S)d-N
0.0775	-5.73427542E-06	4.44208460E-07	(S)H-KKK
0.0776	5.61955528E-06	4.36229992E-07	(S)H-KKN
0.0786	4.45823340E-06	3.50469581E-07	(S)H-KNK
0.0785	-4.39455836E-06	3.45174288E-07	(S)H-KNN
0.2981	2.62367229E-10	7.82155441E-11	(S)H-NNK
0.1216	-1.43911018E-07	1.74998834E-08	(S)H-NNN
0.0175	3.65274202E-07	6.39800778E-09	(S)h-KK
0.1048	9.85442954E-10	1.03293856E-10	(S)h-KN
			(S)h-NN

S' FITTING FOR A MOLECULE WITH K = -0.9,
A TENDENCY = 10^{-2}
WITHOUT USING THE ROTOR PART

Source	Number	Std. Dev.	Scaled
CALC	241	0.0000 Cm-1	0.0004

All	241	0.1635 MHz	0.0004
Ratio	Cm-1	Std. Dev.	
0.0	1.31255412E+01	0.0	A-K
0.0	1.05638418E+01	0.0	A-N
0.0	1.68227617E-01	0.0	a
0.0	-1.00000000E-03	0.0	D-KK
0.0	-1.00000000E-03	0.0	D-KN
0.0	-1.00000000E-03	0.0	D-NN
0.0	-1.00000000E-03	0.0	d-K
0.0	-1.00000000E-03	0.0	d-N
0.0	-1.00000000E-05	0.0	d
0.0	1.00000000E-07	0.0	H-KKK
0.0	1.00000000E-07	0.0	H-KKN
0.0	1.00000000E-07	0.0	H-KNN
0.0	1.00000000E-07	0.0	H-NNN
0.0	1.00000000E-07	0.0	h-KK
0.0	1.00000000E-07	0.0	h-KN
0.0	1.00000000E-07	0.0	h-NN
0.0	1.00000000E-09	0.0	h-K
0.0	1.00000000E-09	0.0	h-N
0.0	1.00000000E-09	0.0	h
0.0000	-2.79064375E-01	4.61319420E-06	(S)A-K
0.0001	-2.35638153E-02	1.26823522E-06	(S)A-N
0.0008	-1.61030809E-03	1.31074613E-06	(S)a'
0.8406	1.38575860E-06	1.16493792E-06	(S)D-KK
0.1419	6.20335932E-04	8.80158781E-05	(S)D-KN
0.1470	-5.90365602E-04	8.67731495E-05	(S)D-NK
0.0069	9.69256084E-06	6.73043387E-08	(S)D-NN
0.0083	1.02794535E-05	8.53243165E-08	(S)d-N
0.1180	2.11038560E-07	2.49082516E-08	(S)d'
0.4923	-3.13386861E-08	1.54265464E-08	(S)H-KKK
0.3970	2.73521418E-06	1.08577664E-06	(S)H-KKN
0.3937	-2.71262981E-06	1.06801669E-06	(S)H-KNK
0.1359	1.45619151E-08	1.97884086E-09	(S)H-NNK
0.1162	2.26485062E-09	2.63253773E-10	(S)H-NNN
0.3701	-2.00771379E-07	7.43142808E-08	(S)h-KN
0.2625	1.14431160E-09	3.00384833E-10	(S)h-NN
0.5569	-3.24032623E-10	1.80458660E-10	(S)h-N

A' FITTING FOR A MOLECULE WITH K = -0.9,
A TENDENCY = 10^{-2} IN THE SPIN-ROTOR PART
WITHOUT USING THE ROTOR PART

Source	Number	Std. Dev.	Scaled
CALC	241	0.0000 Cm-1	0.0006
All	241	0.2705 MHz	0.0006
Ratio	Cm-1	Std. Dev.	
0.0	1.31255412E+01	0.0	A-K
0.0	1.05638418E+01	0.0	A-N
0.0	1.68227617E-01	0.0	a
0.0	-1.00000000E-03	0.0	D-KK
0.0	-1.00000000E-03	0.0	D-KN
0.0	-1.00000000E-03	0.0	D-NN
0.0	-1.00000000E-03	0.0	d-K

0.0	-1.00000000E-03	0.0	d-N
0.0	-1.00000000E-03	0.0	d
0.0	1.00000000E-07	0.0	H-KKK
0.0	1.00000000E-07	0.0	H-KKN
0.0	1.00000000E-07	0.0	H-KNN
0.0	1.00000000E-07	0.0	H-NNN
0.0	1.00000000E-07	0.0	h-KK
0.0	1.00000000E-07	0.0	h-KN
0.0	1.00000000E-07	0.0	h-NN
0.0	1.00000000E-07	0.0	h-K
0.0	1.00000000E-07	0.0	h-N
0.0	1.00000000E-07	0.0	h
0.0000	-2.79075619E-01	4.14122867E-06	(S)A-K
0.0001	-2.35665980E-02	1.62301097E-06	(S)A-N
0.0020	-1.63224170E-03	3.27805233E-06	(S)a'
0.0184	9.54032936E-06	1.75132384E-07	(S)D-KK
0.0115	1.94846203E-05	2.24977865E-07	(S)D-NK
0.0050	1.00402851E-05	5.02610645E-08	(S)D-NN
0.1323	2.15236951E-05	2.84703695E-06	(S)d-K
0.0064	1.01100434E-05	6.51357220E-08	(S)d-N
0.1031	1.27175294E-07	1.31134950E-08	(S)H-KKK
0.1164	-1.07933800E-05	1.25584516E-06	(S)H-KKN
0.1167	1.06364878E-05	1.24125864E-06	(S)H-KNK
0.1084	2.29561454E-06	2.48896361E-07	(S)H-KNN
0.1085	-2.26157823E-06	2.45445930E-07	(S)H-NNK
0.3739	9.53518903E-10	3.56498777E-10	(S)H-NNN
0.3327	-3.50438427E-07	1.16588045E-07	(S)h-KK
0.4991	-3.99609513E-08	1.99426895E-08	(S)h-KN
0.4589	1.08054909E-09	4.95862303E-10	(S)h-NN

S' FITTING FOR A MOLECULE WITH K = -0.9,
A TENDENCY = 10^{-2} IN THE SPIN-ROTOR PART
WITHOUT USING THE ROTOR PART

Source	Number	Std. Dev.	Scaled
CALC	241	0.0000 Cm-1	0.0002
All	241	0.0894 MHz	0.0002
Ratio	Cm-1	Std. Dev.	
0.0	1.31255412E+01	0.0	A-K
0.0	1.05638418E+01	0.0	A-N
0.0	1.68227617E-01	0.0	a
0.0	-1.00000000E-03	0.0	D-KK
0.0	-1.00000000E-03	0.0	D-KN
0.0	-1.00000000E-03	0.0	D-NN
0.0	-1.00000000E-03	0.0	d-K
0.0	-1.00000000E-03	0.0	d-N
0.0	-1.00000000E-03	0.0	d
0.0	1.00000000E-07	0.0	H-KKK
0.0	1.00000000E-07	0.0	H-KKN
0.0	1.00000000E-07	0.0	H-KNN
0.0	1.00000000E-07	0.0	H-NNN
0.0	1.00000000E-07	0.0	h-KK
0.0	1.00000000E-07	0.0	h-KN
0.0	1.00000000E-07	0.0	h-NN

0.0	1.00000000E-07	0.0	h-K
0.0	1.00000000E-07	0.0	h-N
0.0	1.00000000E-07	0.0	h
0.0000	-2.79083992E-01	1.05383746E-06	(S)A-K
0.0000	-2.35673657E-02	4.94129460E-07	(S)A-N
0.0004	-1.61148377E-03	6.95948875E-07	(S)a'
0.0036	9.60363983E-06	3.47530800E-08	(S)D-KK
0.0011	2.06048375E-05	2.34277210E-08	(S)D-NK
0.0014	9.88769444E-06	1.33971430E-08	(S)D-NN
0.0021	1.00953704E-05	2.14135200E-08	(S)d-N
0.0566	1.64585635E-07	9.31698043E-09	(S)d'
0.2481	-1.89298638E-08	4.69698919E-09	(S)H-KKK
0.1744	1.91437112E-06	3.33882408E-07	(S)H-KKN
0.1741	-1.88917651E-06	3.28823886E-07	(S)H-KNK
0.0525	1.63802445E-09	8.60687982E-11	(S)H-NNN
0.0857	1.75314357E-09	1.50294209E-10	(S)h-NN
0.2628	-3.66581984E-10	9.63512988E-11	(S)h-N
0.0288	-7.65212535E-10	2.20181741E-11	(S)h'

A' FITTING FOR A MOLECULE WITH K = -0.9,
A TENDENCY = 10^{-2} IN THE ROTOR PART
WITHOUT USING THE ROTOR PART

Source	Number	Std. Dev.	Scaled
CALC	241	0.0001 Cm-1	0.0104
All	241	4.5961 MHz	0.0108
Ratio	Cm-1	Std. Dev.	
0.0	1.31255412E+01	0.0	A-K
0.0	1.05638418E+01	0.0	A-N
0.0	1.68227617E-01	0.0	a
0.0	-1.00000000E-03	0.0	D-KK
0.0	-1.00000000E-03	0.0	D-KN
0.0	-1.00000000E-03	0.0	D-NN
0.0	-1.00000000E-03	0.0	d-K
0.0	-1.00000000E-03	0.0	d-N
0.0	-1.00000000E-05	0.0	d
0.0	1.00000000E-07	0.0	H-KKK
0.0	1.00000000E-07	0.0	H-KKN
0.0	1.00000000E-07	0.0	H-KNN
0.0	1.00000000E-07	0.0	H-NNN
0.0	1.00000000E-07	0.0	h-KK
0.0	1.00000000E-07	0.0	h-KN
0.0	1.00000000E-07	0.0	h-NN
0.0	1.00000000E-09	0.0	h-K
0.0	1.00000000E-09	0.0	h-N
0.0	1.00000000E-09	0.0	h
0.0003	-2.78673352E-01	8.47866812E-05	(S)A-K
0.0013	-2.40117923E-02	3.16241405E-05	(S)A-N
0.0247	-1.91291873E-03	4.71727424E-05	(S)a'
0.0388	1.65490776E-04	6.41583662E-06	(S)D-KK
0.0483	-8.49986056E-03	4.10144779E-04	(S)D-KN
0.0494	8.32783614E-03	4.11193086E-04	(S)D-NK
0.0248	4.20861947E-05	1.04396454E-06	(S)D-NN
0.1307	3.31417443E-04	4.33077961E-05	(S)d-K

0.0314	-1.76458394E-05	5.54675438E-07	(S)d-N
0.1152	-1.16902301E-06	1.34666952E-07	(S)H-KKK
0.0839	5.38282124E-05	4.51738919E-06	(S)H-KKN
0.0819	-5.29327817E-05	4.33483357E-06	(S)H-KNK
0.6316	4.47645359E-06	2.82717785E-06	(S)H-KNN
0.7162	-4.10166767E-06	2.93749066E-06	(S)H-NNK
0.0908	-7.92288966E-08	7.19051070E-09	(S)H-NNN
0.1612	-1.42938958E-05	2.30459016E-06	(S)h-KK
0.0128	3.76036256E-05	4.81721684E-07	(S)h-KN

S' FITTING FOR A MOLECULE WITH K = -0.9,
A TENDENCY = 10^{-2} IN THE ROTOR PART
WITHOUT USING THE ROTOR PART

Source	Number	Std. Dev.	Scaled
CALC	241	0.0000 Cm-1	0.0004
All	241	0.1714 MHz	0.0004
Ratio	Cm-1	Std. Dev.	
0.0	1.31255412E+01	0.0	A-K
0.0	1.05638418E+01	0.0	A-N
0.0	1.68227617E-01	0.0	a
0.0	-1.00000000E-03	0.0	D-KK
0.0	-1.00000000E-03	0.0	D-KN
0.0	-1.00000000E-03	0.0	D-NN
0.0	-1.00000000E-03	0.0	d-K
0.0	-1.00000000E-03	0.0	d-N
0.0	-1.00000000E-05	0.0	d
0.0	1.00000000E-07	0.0	H-KKK
0.0	1.00000000E-07	0.0	H-KKN
0.0	1.00000000E-07	0.0	H-KNN
0.0	1.00000000E-07	0.0	H-NNN
0.0	1.00000000E-07	0.0	h-KK
0.0	1.00000000E-07	0.0	h-KN
0.0	1.00000000E-07	0.0	h-NN
0.0	1.00000000E-09	0.0	h-K
0.0	1.00000000E-09	0.0	h-N
0.0	1.00000000E-09	0.0	h
0.0000	-2.79145961E-01	3.50448179E-06	(S)A-K
0.0001	-2.35639297E-02	1.37470449E-06	(S)A-N
0.0009	-1.60357330E-03	1.37087346E-06	(S)a'
0.0213	2.95637282E-05	6.29994818E-07	(S)D-KK
0.0246	-1.61917636E-03	3.98601458E-05	(S)D-KN
0.0243	1.61758050E-03	3.92568524E-05	(S)D-NK
0.0078	9.57436524E-06	7.50316207E-08	(S)D-NN
0.0047	2.02308148E-05	9.57997681E-08	(S)d-N
0.0027	1.01857205E-05	2.71858593E-08	(S)d'
0.1845	3.55394299E-08	6.55534707E-09	(S)H-KKK
0.1569	-3.25816865E-06	5.11178627E-07	(S)H-KKN
0.1605	3.15693364E-06	5.06733184E-07	(S)H-KNK
0.0247	8.29830245E-08	2.05053110E-09	(S)H-NNK
0.0986	2.83631631E-09	2.79570719E-10	(S)H-NNN
0.3859	-2.20908572E-07	8.52523277E-08	(S)h-KN
0.1540	2.04516156E-09	3.14940626E-10	(S)h-NN
0.1707	1.11227343E-09	1.89876514E-10	(S)h-N

0.0427	9.86376052E-10	4.21442599E-11	(S)h'

A' FITTING FOR A MOLECULE WITH K = -0.9,
WITHOUT A TENDENCY
WITHOUT USING THE ROTOR PART

Source	Number	Std. Dev.	Scaled
CALC	241	0.0009 Cm-1	0.0646
All	241	28.2679 MHz	0.0665
Ratio	Cm-1	Std. Dev.	
0.0	1.31255412E+01	0.0	A-K
0.0	1.05638418E+01	0.0	A-N
0.0	1.68227617E-01	0.0	a
0.0	-1.00000000E-03	0.0	D-KK
0.0	-1.00000000E-03	0.0	D-KN
0.0	-1.00000000E-03	0.0	D-NN
0.0	-1.00000000E-03	0.0	d-K
0.0	-1.00000000E-03	0.0	d-N
0.0	-1.00000000E-03	0.0	d
0.0	1.00000000E-07	0.0	H-KKK
0.0	1.00000000E-07	0.0	H-KKN
0.0	1.00000000E-07	0.0	H-KNN
0.0	1.00000000E-07	0.0	H-NNN
0.0	1.00000000E-07	0.0	h-KK
0.0	1.00000000E-07	0.0	h-KN
0.0	1.00000000E-07	0.0	h-NN
0.0	1.00000000E-07	0.0	h-K
0.0	1.00000000E-07	0.0	h-N
0.0	1.00000000E-07	0.0	h
0.0012	-2.78368590E-01	3.20622489E-04	(S)A-K
0.0041	-2.36042355E-02	9.62333990E-05	(S)A-N
0.0762	-2.32438250E-03	1.77005741E-04	(S)a'
0.7252	1.19010419E-03	8.63090681E-04	(S)D-KN
0.7111	-1.20383821E-03	8.55990970E-04	(S)D-NK
0.0848	1.47710522E-05	1.25283441E-06	(S)D-NN
0.1841	8.40957625E-04	1.54857270E-04	(S)d-K
0.0890	1.71292649E-05	1.52402146E-06	(S)d-N
0.9930	4.60198240E-07	4.56974318E-07	(S)H-KKK
0.0942	-1.14766886E-04	1.08057974E-05	(S)H-KKN
0.0962	1.14571676E-04	1.10176585E-05	(S)H-KNK
0.3068	2.41573965E-05	7.41219993E-06	(S)H-KNN
0.3064	-2.39896760E-05	7.34963943E-06	(S)H-NNK
0.2149	-3.85780636E-05	8.29030326E-06	(S)h-KK

S' FITTING FOR A MOLECULE WITH K = -0.9,
WITHOUT A TENDENCY
WITHOUT USING THE ROTOR PART

Source	Number	Std. Dev.	Scaled
CALC	241	0.0000 Cm-1	0.0013
All	241	0.5740 MHz	0.0014
Ratio	Cm-1	Std. Dev.	
0.0	1.31255412E+01	0.0	A-K
0.0	1.05638418E+01	0.0	A-N

0.0	1.68227617E-01	0.0	a
0.0	-1.00000000E-03	0.0	D-KK
0.0	-1.00000000E-03	0.0	D-KN
0.0	-1.00000000E-03	0.0	D-NN
0.0	-1.00000000E-03	0.0	d-K
0.0	-1.00000000E-03	0.0	d-N
0.0	-1.00000000E-03	0.0	d
0.0	1.00000000E-07	0.0	H-KKK
0.0	1.00000000E-07	0.0	H-KKN
0.0	1.00000000E-07	0.0	H-KNN
0.0	1.00000000E-07	0.0	H-NNN
0.0	1.00000000E-07	0.0	h-KK
0.0	1.00000000E-07	0.0	h-KN
0.0	1.00000000E-07	0.0	h-NN
0.0	1.00000000E-07	0.0	h-K
0.0	1.00000000E-07	0.0	h-N
0.0	1.00000000E-07	0.0	h
0.0000	-2.79079279E-01	7.07181643E-06	(S)A-K
0.0001	-2.35700030E-02	3.16492098E-06	(S)A-N
0.0028	-1.60177962E-03	4.46874746E-06	(S)a'
0.0205	9.07121867E-06	1.86311707E-07	(S)D-KK
0.0088	2.11646737E-05	1.85405458E-07	(S)D-NK
0.0087	9.85857751E-06	8.58461536E-08	(S)D-NN
0.0069	1.99696127E-05	1.37509900E-07	(S)d-N
0.0059	1.01297089E-05	5.98235954E-08	(S)d'
0.4181	-5.97152195E-08	2.49672792E-08	(S)H-KKK
0.3020	5.33018329E-06	1.60985407E-06	(S)H-KKN
0.3008	-5.25853890E-06	1.58178936E-06	(S)H-KNK
0.3295	1.67214882E-09	5.50989367E-10	(S)H-NNN
0.2712	3.55853541E-09	9.65085307E-10	(S)h-NN
0.4735	1.30654931E-09	6.18687545E-10	(S)h-N
0.2620	-5.39604741E-10	1.41400759E-10	(S)h'

A FITTING FOR A MOLECULE WITH K = -0.5,
A TENDENCY = 10^{-2}
WITH ALL THE SPIN-ROTOR PARAMETERS

Source	Number	Std. Dev.	Scaled
CALC	241	0.0001 Cm-1	0.0074
All	241	3.2337 MHz	0.0076
Ratio	Cm-1	Std. Dev.	
0.0000	1.31254009E+01	3.76717873E-06	A-K
0.0000	1.05638820E+01	1.63789678E-06	A-N
0.0000	9.34999934E-01	1.78960543E-06	a
0.0002	-1.09868622E-03	1.95273605E-07	D-KK
0.0003	-8.80814564E-04	2.36067393E-07	D-KN
0.0001	-1.01996777E-03	5.42825857E-08	D-NN
0.0004	-1.28342036E-03	5.07324147E-07	d-K
0.0000	-9.99594382E-04	4.60514619E-08	d-N
0.0150	5.34698837E-07	8.00049107E-09	H-KKK
0.0226	-5.05422713E-07	1.14007274E-08	H-KKN
0.0150	2.71009202E-07	4.05181274E-09	H-KNN
0.0042	1.01968911E-07	4.23223506E-10	H-NNN
0.0260	7.50099222E-07	1.95272240E-08	h-KK

0.0227	-2.13842784E-07	4.86452928E-09	h-KN
0.0029	1.00218435E-07	2.88777832E-10	h-NN
0.0	-2.79083130E-01	0.0	(S)A-K
0.0	-2.35670735E-02	0.0	(S)A-N
0.0	-9.00985622E-03	0.0	(S)a'
0.0	1.00000000E-05	0.0	(S)D-KK
0.0	1.00000000E-05	0.0	(S)D-KN
0.0	1.00000000E-05	0.0	(S)D-NK
0.0	1.00000000E-05	0.0	(S)D-NN
0.0	1.00000000E-05	0.0	(S)d-K
0.0	1.00000000E-07	0.0	(S)d-K'
0.0	1.00000000E-05	0.0	(S)d-N
0.0	1.00000000E-07	0.0	(S)d-N'
0.0	1.00000000E-07	0.0	(S)d'
0.0	1.00000000E-09	0.0	(S)H-KKK
0.0	1.00000000E-09	0.0	(S)H-KKN
0.0	1.00000000E-09	0.0	(S)H-KNK
0.0	1.00000000E-09	0.0	(S)H-KNN
0.0	1.00000000E-09	0.0	(S)H-NNK
0.0	1.00000000E-09	0.0	(S)H-NNN
0.0	1.00000000E-09	0.0	(S)h-KK
0.0	1.00000000E-11	0.0	(S)h-KK'
0.0	1.00000000E-09	0.0	(S)h-KN
0.0	1.00000000E-11	0.0	(S)h-NK
0.0	1.00000000E-11	0.0	(S)h-NK'
0.0	1.00000000E-09	0.0	(S)h-NN
0.0	1.00000000E-11	0.0	(S)h-NN'
0.0	1.00000000E-11	0.0	(S)h-K
0.0	1.00000000E-11	0.0	(S)h-K'
0.0	1.00000000E-11	0.0	(S)h-N
0.0	1.00000000E-11	0.0	(S)h-N'
0.0	1.00000000E-11	0.0	(S)h'

S FITTING FOR A MOLECULE WITH K = -0.5,
A TENDENCY = 10^{-2}
WITH ALL THE SPIN-ROTOR PARAMETERS

Source	Number	Std. Dev.	Scaled
CALC	241	0.0000 Cm-1	0.0011
All	241	0.4612 MHz	0.0011
Ratio	Cm-1	Std. Dev.	
0.0000	1.31260333E+01	5.35062460E-07	A-K
0.0000	1.05637016E+01	2.33059480E-07	A-N
0.0000	9.33719903E-01	2.43340335E-07	a
0.0000	-6.45462388E-04	1.58517422E-08	D-KK
0.0000	-1.42638677E-03	2.00753249E-08	D-KN
0.0000	-9.28821473E-04	6.35503319E-09	D-NN
0.0000	-9.99892721E-04	6.48612515E-09	d-N
0.0001	-4.55375622E-05	2.27801430E-09	d
0.0008	-1.48304585E-07	1.14929496E-10	H-KKK
0.0031	7.29407434E-08	2.28650184E-10	H-KKN
0.0004	4.50617213E-07	1.76920579E-10	H-KNN
0.0017	2.40526448E-08	4.16982332E-11	H-NNN
0.0004	9.84309868E-08	4.11400551E-11	h-NN

0.0006	3.91561795E-08	2.26689710E-11	h-N
0.0018	2.61978751E-09	4.66304860E-12	h
0.0	-2.79083130E-01	0.0	(S)A-K
0.0	-2.35670735E-02	0.0	(S)A-N
0.0	-9.00985622E-03	0.0	(S)a'
0.0	1.00000000E-05	0.0	(S)D-KK
0.0	1.00000000E-05	0.0	(S)D-KN
0.0	1.00000000E-05	0.0	(S)D-NK
0.0	1.00000000E-05	0.0	(S)D-NN
0.0	1.00000000E-05	0.0	(S)d-K
0.0	1.00000000E-07	0.0	(S)d-K'
0.0	1.00000000E-05	0.0	(S)d-N
0.0	1.00000000E-07	0.0	(S)d-N'
0.0	1.00000000E-07	0.0	(S)d'
0.0	1.00000000E-09	0.0	(S)H-KKK
0.0	1.00000000E-09	0.0	(S)H-KKN
0.0	1.00000000E-09	0.0	(S)H-KNK
0.0	1.00000000E-09	0.0	(S)H-KNN
0.0	1.00000000E-09	0.0	(S)H-NNK
0.0	1.00000000E-09	0.0	(S)H-NNN
0.0	1.00000000E-09	0.0	(S)h-KK
0.0	1.00000000E-11	0.0	(S)h-KK'
0.0	1.00000000E-09	0.0	(S)h-KN
0.0	1.00000000E-11	0.0	(S)h-NK
0.0	1.00000000E-11	0.0	(S)h-NK'
0.0	1.00000000E-09	0.0	(S)h-NN
0.0	1.00000000E-11	0.0	(S)h-NN'
0.0	1.00000000E-11	0.0	(S)h-K
0.0	1.00000000E-11	0.0	(S)h-K'
0.0	1.00000000E-11	0.0	(S)h-N
0.0	1.00000000E-11	0.0	(S)h-N'
0.0	1.00000000E-11	0.0	(S)h'

A FITTING FOR A MOLECULE WITH K = -0.5,
A TENDENCY = 10^{-2} IN THE SPIN-ROTOR
WITH ALL THE SPIN-ROTOR PARAMETERS

Source	Number	Std. Dev.	Scaled
CALC	241	0.1671 Cm-1	11.7907
All	241	5172.6110 MHz	12.1757
Ratio	Cm-1	Std. Dev.	
0.0005	1.31076820E+01	6.21252988E-03	A-K
0.0003	1.05691145E+01	2.67101877E-03	A-N
0.0029	9.67164375E-01	2.75862121E-03	a
0.0212	-1.10053723E-02	2.33247952E-04	D-KK
0.0198	1.17799051E-02	2.32922939E-04	D-KN
0.0217	-3.24432835E-03	7.04022661E-05	D-NN
0.0161	-3.24801817E-02	5.23400400E-04	d-K
0.0709	-1.03518397E-03	7.33651109E-05	d-N
0.0099	2.87992841E-04	2.85559135E-06	H-KKK
0.0123	-3.98693001E-04	4.89474648E-06	H-KKN
0.0226	1.08286228E-04	2.45023463E-06	H-KNN
0.1693	2.66862413E-06	4.51765436E-07	H-NNN
0.1015	2.43081798E-05	2.46636365E-06	h-KK

0.3287	-1.56349012E-05	5.13928069E-06	h-KN
0.3929	1.20226454E-06	4.72318237E-07	h-NN
0.0	-2.79083130E-01	0.0	(S)A-K
0.0	-2.35670735E-02	0.0	(S)A-N
0.0	-9.00985622E-03	0.0	(S)a'
0.0	1.00000000E-05	0.0	(S)D-KK
0.0	1.00000000E-05	0.0	(S)D-KN
0.0	1.00000000E-05	0.0	(S)D-NK
0.0	1.00000000E-05	0.0	(S)D-NN
0.0	1.00000000E-05	0.0	(S)d-K
0.0	1.00000000E-07	0.0	(S)d-K'
0.0	1.00000000E-05	0.0	(S)d-N
0.0	1.00000000E-07	0.0	(S)d-N'
0.0	1.00000000E-07	0.0	(S)d'
0.0	1.00000000E-09	0.0	(S)H-KKK
0.0	1.00000000E-09	0.0	(S)H-KKN
0.0	1.00000000E-09	0.0	(S)H-KNK
0.0	1.00000000E-09	0.0	(S)H-KNN
0.0	1.00000000E-09	0.0	(S)H-NNK
0.0	1.00000000E-09	0.0	(S)H-NNN
0.0	1.00000000E-09	0.0	(S)h-KK
0.0	1.00000000E-11	0.0	(S)h-KK'
0.0	1.00000000E-09	0.0	(S)h-KN
0.0	1.00000000E-11	0.0	(S)h-NK
0.0	1.00000000E-11	0.0	(S)h-NK'
0.0	1.00000000E-09	0.0	(S)h-NN
0.0	1.00000000E-11	0.0	(S)h-NN'
0.0	1.00000000E-11	0.0	(S)h-K
0.0	1.00000000E-11	0.0	(S)h-K'
0.0	1.00000000E-11	0.0	(S)h-N
0.0	1.00000000E-11	0.0	(S)h-N'
0.0	1.00000000E-11	0.0	(S)h'

S FITTING FOR A MOLECULE WITH K = -0.5,
A TENDENCY = 10^{-2} IN THE SPIN-ROTOR
WITH ALL THE SPIN-ROTOR PARAMETERS

Source	Number	Std. Dev.	Scaled
CALC	241	0.0003 Cm-1	0.0199
All	241	8.7185 MHz	0.0205
Ratio	Cm-1	Std. Dev.	
0.0000	1.31260197E+01	1.00964608E-05	A-K
0.0000	1.05637059E+01	4.40095317E-06	A-N
0.0000	9.33726427E-01	4.54895982E-06	a
0.0005	-6.45580202E-04	2.95948047E-07	D-KK
0.0003	-1.42589544E-03	3.75519530E-07	D-KN
0.0001	-9.28956671E-04	1.19756490E-07	D-NN
0.0001	-9.99744548E-04	1.20733598E-07	d-N
0.0000	-1.03517165E-03	4.28588982E-08	d
0.1760	1.19940596E-08	2.11105508E-09	H-KKK
0.0151	-2.77825697E-07	4.20366755E-09	H-KKN
0.0049	6.65150101E-07	3.27948067E-09	H-KNN
3.2660	-2.39916804E-10	7.83566296E-10	H-NNN
0.0258	2.96164433E-08	7.62822870E-10	h-NN

0.0028	1.52515919E-07	4.26825845E-10	h-N
0.0005	1.73804331E-07	8.74712384E-11	h
0.0	-2.79083130E-01	0.0	(S)A-K
0.0	-2.35670735E-02	0.0	(S)A-N
0.0	-9.00985622E-03	0.0	(S)a'
0.0	1.00000000E-05	0.0	(S)D-KK
0.0	1.00000000E-05	0.0	(S)D-KN
0.0	1.00000000E-05	0.0	(S)D-NK
0.0	1.00000000E-05	0.0	(S)D-NN
0.0	1.00000000E-05	0.0	(S)d-K
0.0	1.00000000E-07	0.0	(S)d-K'
0.0	1.00000000E-05	0.0	(S)d-N
0.0	1.00000000E-07	0.0	(S)d-N'
0.0	1.00000000E-07	0.0	(S)d'
0.0	1.00000000E-09	0.0	(S)H-KKK
0.0	1.00000000E-09	0.0	(S)H-KKN
0.0	1.00000000E-09	0.0	(S)H-KNK
0.0	1.00000000E-09	0.0	(S)H-KNN
0.0	1.00000000E-09	0.0	(S)H-NNK
0.0	1.00000000E-09	0.0	(S)H-NNN
0.0	1.00000000E-09	0.0	(S)h-KK
0.0	1.00000000E-09	0.0	(S)h-KK'
0.0	1.00000000E-11	0.0	(S)h-KN
0.0	1.00000000E-09	0.0	(S)h-NK
0.0	1.00000000E-11	0.0	(S)h-NK'
0.0	1.00000000E-11	0.0	(S)h-NN
0.0	1.00000000E-09	0.0	(S)h-NN'
0.0	1.00000000E-11	0.0	(S)h-K
0.0	1.00000000E-11	0.0	(S)h-K'
0.0	1.00000000E-11	0.0	(S)h-N
0.0	1.00000000E-11	0.0	(S)h-N'
0.0	1.00000000E-11	0.0	(S)h'
0.0	1.00000000E-11	0.0	

A FITTING FOR A MOLECULE WITH K = -0.5,
A TENDENCY = 10^{-2} IN THE ROTOR PART
WITH ALL THE SPIN-ROTOR PARAMETERS

Source	Number	Std. Dev.	Scaled
CALC	241	0.0001 Cm-1	0.0074
All	241	3.2635 MHz	0.0077
Ratio	Cm-1	Std. Dev.	
0.0000	1.31254010E+01	3.80184043E-06	A-K
0.0000	1.05638819E+01	1.65296505E-06	A-N
0.0000	9.34999945E-01	1.80607301E-06	a
0.0002	-1.09868004E-03	1.97071843E-07	D-KK
0.0003	-8.80822738E-04	2.38243404E-07	D-KN
0.0001	-1.01996607E-03	5.47826699E-08	D-NN
0.0004	-1.28345603E-03	5.11961535E-07	d-K
0.0000	-9.99593847E-04	4.64754450E-08	d-N
0.0150	5.37100185E-07	8.07475747E-09	H-KKK
0.0226	-5.08804375E-07	1.15066889E-08	H-KKN
0.0150	2.72038067E-07	4.08937520E-09	H-KNN
0.0042	1.01958601E-07	4.27124340E-10	H-NNN
0.0261	7.56119748E-07	1.97060042E-08	h-KK

0.0230	-2.13783099E-07	4.90892876E-09	h-KN
0.0029	1.00213799E-07	2.91437656E-10	h-NN
0.0	-2.79083130E-01	0.0	(S)A-K
0.0	-2.35670735E-02	0.0	(S)A-N
0.0	-9.00985622E-03	0.0	(S)a'
0.0	1.00000000E-05	0.0	(S)D-KK
0.0	1.00000000E-05	0.0	(S)D-KN
0.0	1.00000000E-05	0.0	(S)D-NK
0.0	1.00000000E-05	0.0	(S)D-NN
0.0	1.00000000E-05	0.0	(S)d-K
0.0	1.00000000E-05	0.0	(S)d-K'
0.0	1.00000000E-05	0.0	(S)d-N
0.0	1.00000000E-05	0.0	(S)d-N'
0.0	1.00000000E-05	0.0	(S)d'
0.0	1.00000000E-09	0.0	(S)H-KKK
0.0	1.00000000E-09	0.0	(S)H-KKN
0.0	1.00000000E-09	0.0	(S)H-KNK
0.0	1.00000000E-09	0.0	(S)H-KNN
0.0	1.00000000E-09	0.0	(S)H-NNK
0.0	1.00000000E-09	0.0	(S)H-NNN
0.0	1.00000000E-09	0.0	(S)h-KK
0.0	1.00000000E-09	0.0	(S)h-KK'
0.0	1.00000000E-09	0.0	(S)h-KN
0.0	1.00000000E-09	0.0	(S)h-NK
0.0	1.00000000E-09	0.0	(S)h-NK'
0.0	1.00000000E-09	0.0	(S)h-NN
0.0	1.00000000E-09	0.0	(S)h-NN'
0.0	1.00000000E-09	0.0	(S)h-K
0.0	1.00000000E-09	0.0	(S)h-K'
0.0	1.00000000E-09	0.0	(S)h-N
0.0	1.00000000E-09	0.0	(S)h-N'
0.0	1.00000000E-09	0.0	(S)h'

S FITTING FOR A MOLECULE WITH K = -0.5,
A TENDENCY = 10^{-2} IN THE ROTOR PART
WITH ALL THE SPIN-ROTOR PARAMETERS

Source	Number	Std. Dev.	Scaled
CALC	241	0.0000 Cm-1	0.0011
All	241	0.4720 MHz	0.0011
Ratio	Cm-1	Std. Dev.	
0.0000	1.31260333E+01	5.47489392E-07	A-K
0.0000	1.05637016E+01	2.38471628E-07	A-N
0.0000	9.33719887E-01	2.48991162E-07	a
0.0000	-6.45449750E-04	1.62201895E-08	D-KK
0.0000	-1.42640269E-03	2.05418727E-08	D-KN
0.0000	-9.28818948E-04	6.50262713E-09	D-NN
0.0000	-9.99891273E-04	6.63675514E-09	d-N
0.0001	-4.55387454E-05	2.33089557E-09	d
0.0008	-1.48112197E-07	1.17602930E-10	H-KKK
0.0032	7.27928952E-08	2.33969831E-10	H-KKN
0.0004	4.50556785E-07	1.81035185E-10	H-KNN
0.0018	2.40768798E-08	4.26668789E-11	H-NNN
0.0004	9.84508903E-08	4.20955612E-11	h-NN

0.0006	3.91437265E-08	2.31951898E-11	h-N
0.0018	2.58430344E-09	4.77128534E-12	h
0.0	-2.79083130E-01	0.0	(S)A-K
0.0	-2.35670735E-02	0.0	(S)A-N
0.0	-9.00985622E-03	0.0	(S)a'
0.0	1.00000000E-05	0.0	(S)D-KK
0.0	1.00000000E-05	0.0	(S)D-KN
0.0	1.00000000E-05	0.0	(S)D-NK
0.0	1.00000000E-05	0.0	(S)D-NN
0.0	1.00000000E-05	0.0	(S)d-K
0.0	1.00000000E-05	0.0	(S)d-K'
0.0	1.00000000E-05	0.0	(S)d-N
0.0	1.00000000E-05	0.0	(S)d-N'
0.0	1.00000000E-05	0.0	(S)d'
0.0	1.00000000E-09	0.0	(S)H-KKK
0.0	1.00000000E-09	0.0	(S)H-KKN
0.0	1.00000000E-09	0.0	(S)H-KNK
0.0	1.00000000E-09	0.0	(S)H-KNN
0.0	1.00000000E-09	0.0	(S)H-NNK
0.0	1.00000000E-09	0.0	(S)H-NNN
0.0	1.00000000E-09	0.0	(S)h-KK
0.0	1.00000000E-09	0.0	(S)h-KK'
0.0	1.00000000E-09	0.0	(S)h-KN
0.0	1.00000000E-09	0.0	(S)h-NK
0.0	1.00000000E-09	0.0	(S)h-NK'
0.0	1.00000000E-09	0.0	(S)h-NN
0.0	1.00000000E-09	0.0	(S)h-NN'
0.0	1.00000000E-09	0.0	(S)h-K
0.0	1.00000000E-09	0.0	(S)h-K'
0.0	1.00000000E-09	0.0	(S)h-N
0.0	1.00000000E-09	0.0	(S)h-N'
0.0	1.00000000E-09	0.0	(S)h'

A FITTING FOR A MOLECULE WITH K = -0.5,
A TENDENCY = 10^{-2}
WITH THE SECOND ORDER OF MAGNITUDE SPIN-ROTOR PARAMETERS

Source	Number	Std. Dev.	Scaled
CALC	241	0.0001 Cm-1	0.0074
All	241	3.2515 MHz	0.0077
Ratio	Cm-1	Std. Dev.	
0.0000	1.31253993E+01	2.00119053E-05	A-K
0.0000	1.05638824E+01	8.69105026E-06	A-N
0.0000	9.34992966E-01	8.66496148E-06	a
0.0002	-1.09868609E-03	1.96491294E-07	D-KK
0.0004	-8.80796573E-04	3.11806944E-07	D-KN
0.0001	-1.01997315E-03	1.05696306E-07	D-NN
0.0004	-1.28343059E-03	5.10792884E-07	d-K
0.0001	-9.99519259E-04	1.02210859E-07	d-N
0.0151	5.34745324E-07	8.04966945E-09	H-KKK
0.0227	-5.05493134E-07	1.14681481E-08	H-KKN
0.0155	2.70952385E-07	4.18926829E-09	H-KNN
0.0057	1.01993707E-07	5.79609397E-10	H-NNN
0.0262	7.50034814E-07	1.96484475E-08	h-KK

0.0229	-2.13912257E-07	4.89476337E-09	h-KN
0.0050	9.98871578E-08	4.95751914E-10	h-NN
0.0006	-2.79069345E-01	1.67271651E-04	(S)A-K
0.0031	-2.35708623E-02	7.29772465E-05	(S)A-N
0.0081	-8.95030025E-03	7.24983330E-05	(S)a'

S FITTING FOR A MOLECULE WITH K = -0.5,
A TENDENCY = 10^{-2}
WITH THE SECOND ORDER OF MAGNITUDE SPIN-ROTOR PARAMETERS

CALC	241	0.0000 Cm-1	0.0010
All	241	0.4514 MHz	0.0011
Ratio	Cm-1	Std. Dev.	
0.0000	1.31260247E+01	2.77461810E-06	A-K
0.0000	1.05637049E+01	1.20543391E-06	A-N
0.0000	9.33721840E-01	1.20022802E-06	a
0.0000	-6.45470163E-04	1.55190666E-08	D-KK
0.0000	-1.42628559E-03	3.49861526E-08	D-KN
0.0000	-9.28858745E-04	1.41094451E-08	D-NN
0.0000	-9.99913481E-04	1.41364977E-08	d-N
0.0000	-4.55366453E-05	2.23035089E-09	d
0.0008	-1.48541622E-07	1.12486216E-10	H-KKK
0.0031	7.31901001E-08	2.23832236E-10	H-KKN
0.0005	4.50211672E-07	2.15029501E-10	H-KNN
0.0029	2.41935022E-08	6.90165018E-11	H-NNN
0.0007	9.85226770E-08	6.86893252E-11	h-NN
0.0006	3.91636206E-08	2.21917245E-11	h-N
0.0017	2.61983272E-09	4.56374239E-12	h
0.0001	-2.79010905E-01	2.32070893E-05	(S)A-K
0.0004	-2.35955480E-02	1.01262588E-05	(S)A-N
0.0011	-9.02647921E-03	1.00479850E-05	(S)a'

A FITTING FOR A MOLECULE WITH K = -0.5,
WITHOUT A TENDENCY
WITH THE SECOND ORDER OF MAGNITUDE SPIN-ROTOR PARAMETERS

Source	Number	Std. Dev.	Scaled
CALC	241	0.1695 Cm-1	11.9595
All	241	5235.0902 MHz	12.3227
Ratio	Cm-1	Std. Dev.	
0.0005	1.31107996E+01	6.16069231E-03	A-K
0.0003	1.05680722E+01	2.67042212E-03	A-N
0.0015	9.61089829E-01	1.39932788E-03	a
0.0213	-1.10515419E-02	2.35283950E-04	D-KK
0.0200	1.17409571E-02	2.35208843E-04	D-KN
0.0219	-3.22208280E-03	7.06913366E-05	D-NN
0.0157	-3.27820886E-02	5.15518274E-04	d-K
0.0178	-8.52383394E-04	1.51981009E-05	d-N
0.0100	2.87957800E-04	2.89076339E-06	H-KKK
0.0124	-3.98209428E-04	4.95092945E-06	H-KKN
0.0229	1.08358211E-04	2.48049100E-06	H-KNN
0.1782	2.55290720E-06	4.54855717E-07	H-NNN
0.1039	2.39902348E-05	2.49269930E-06	h-KK
0.4025	-1.25495015E-05	1.05149941E-06	h-KN

0.0	-2.79083130E-01	0.0	(S)A-K
0.0	-2.35670735E-02	0.0	(S)A-N
0.0	-9.00985622E-03	0.0	(S)a'

S FITTING FOR A MOLECULE WITH K = -0.5,
WITHOUT A TENDENCY
WITH THE SECOND ORDER OF MAGNITUDE SPIN-ROTOR PARAMETERS

CALC	241	0.0003 Cm-1	0.0199
All	241	8.7733 MHz	0.0207
Ratio	Cm-1	Std. Dev.	
0.0000	1.31259995E+01	5.37728493E-05	A-K
0.0000	1.05637121E+01	2.35312079E-05	A-N
0.0000	9.33731217E-01	2.26869425E-05	a
0.0005	-6.45585541E-04	2.97911767E-07	D-KK
0.0005	-1.42567102E-03	6.74443967E-07	D-KN
0.0003	-9.29024359E-04	2.75230650E-07	D-NN
0.0003	-9.99795572E-04	2.66964239E-07	d-N
0.0000	-1.03517023E-03	4.31713774E-08	d
0.1805	1.17678501E-08	2.12436699E-09	H-KKK
0.0152	-2.77609137E-07	4.23062213E-09	H-KKN
0.0062	6.64214102E-07	4.09707627E-09	H-KNN
0.1139	3.34548206E-11	1.34200242E-09	H-NNN
0.0434	2.98386431E-08	1.29356244E-09	h-NN
0.0028	1.52517575E-07	4.29907992E-10	h-N
0.0005	1.73803331E-07	8.81116240E-11	h
0.0016	-2.78911321E-01	4.49601244E-04	(S)A-K
0.0084	-2.36200787E-02	1.97490812E-04	(S)A-N
0.0210	-9.05090392E-03	1.89866545E-04	(S)a'

A FITTING FOR A MOLECULE WITH K = -0.5,
A TENDENCY = 10^{-2}
WITHOUT THE SPIN-ROTOR PARAMETERS

Source	Number	Std. Dev.	Scaled
CALC	241	0.0001 Cm-1	0.0074
All	241	3.2323 MHz	0.0076
Ratio	Cm-1	Std. Dev.	
0.0000	1.31254004E+01	3.76525826E-06	A-K
0.0000	1.05638822E+01	1.63712305E-06	A-N
0.0000	9.35000230E-01	1.78919800E-06	a
0.0002	-1.09868776E-03	1.95202022E-07	D-KK
0.0003	-8.80798121E-04	2.35992762E-07	D-KN
0.0001	-1.01997467E-03	5.42627811E-08	D-NN
0.0004	-1.28370916E-03	5.07519851E-07	d-K
0.0000	-9.99596019E-04	4.60383448E-08	d-N
0.0150	5.34681701E-07	8.00138391E-09	H-KKK
0.0226	-5.05402547E-07	1.14017431E-08	H-KKN
0.0150	2.70910391E-07	4.05152443E-09	H-KNN
0.0041	1.02012993E-07	4.23079944E-10	H-NNN
0.0260	7.50237723E-07	1.95403322E-08	h-KK
0.0229	-2.12764213E-07	4.86632231E-09	h-KN
0.0029	1.00221639E-07	2.88691201E-10	h-NN

S FITTING FOR A MOLECULE WITH K = -0.5,
A TENDENCY = 10^{-2}
WITHOUT THE SPIN-ROTOR PARAMETERS

Source	Number	Std. Dev.	Scaled
CALC	241	0.0000 Cm-1	0.0007
All	241	0.3148 MHz	0.0007
Ratio	Cm-1	Std. Dev.	
0.0000	1.31260345E+01	3.65108335E-07	A-K
0.0000	1.05637010E+01	1.59037929E-07	A-N
0.0000	9.33719923E-01	1.66088552E-07	a
0.0000	-6.45802471E-04	1.08157307E-08	D-KK
0.0000	-1.42602984E-03	1.36979464E-08	D-KN
0.0000	-9.28866736E-04	4.33660079E-09	D-NN
0.0000	-9.99892261E-04	4.42693321E-09	d-N
0.0000	-4.55034056E-05	1.55476546E-09	d
0.0005	-1.48473274E-07	7.84136898E-11	H-KKK
0.0021	7.47714182E-08	1.55999219E-10	H-KKN
0.0003	4.48978159E-07	1.20709366E-10	H-KNN
0.0012	2.42158451E-08	2.84537627E-11	H-NNN
0.0003	9.84295688E-08	2.80785173E-11	h-NN
0.0004	3.90011699E-08	1.54716969E-11	h-N
0.0012	2.62073045E-09	3.18244796E-12	h

A FITTING FOR A MOLECULE WITH K = -0.5,
WITHOUT A TENDENCY
WITHOUT THE SPIN-ROTOR PARAMETERS

Source	Number	Std. Dev.	Scaled
CALC	241	0.1669 Cm-1	11.7779
All	241	5167.0053 MHz	12.1625
Ratio	Cm-1	Std. Dev.	
0.0005	1.31076641E+01	6.20536637E-03	A-K
0.0003	1.05691201E+01	2.66802716E-03	A-N
0.0028	9.67185078E-01	2.75611868E-03	a
0.0212	-1.10050540E-02	2.32980673E-04	D-KK
0.0198	1.17800657E-02	2.32662744E-04	D-KN
0.0217	-3.24446836E-03	7.03248202E-05	D-NN
0.0161	-3.25092153E-02	5.23074119E-04	d-K
0.0708	-1.03510108E-03	7.32973535E-05	d-N
0.0099	2.88029076E-04	2.85290058E-06	H-KKK
0.0123	-3.98749488E-04	4.88985019E-06	H-KKN
0.0226	1.08303807E-04	2.44759053E-06	H-KNN
0.1691	2.66923671E-06	4.51268565E-07	H-NNN
0.1014	2.42921467E-05	2.46440998E-06	h-KK
0.3309	-1.55205817E-05	5.13588099E-06	h-KN
0.3929	1.20089119E-06	4.71877358E-07	h-NN

S FITTING FOR A MOLECULE WITH K = -0.5,
WITHOUT A TENDENCY
WITHOUT THE SPIN-ROTOR PARAMETERS

Source	Number	Std. Dev.	Scaled
CALC	241	0.0003 Cm-1	0.0200
All	241	8.7612 MHz	0.0206

Ratio	Cm-1	Std. Dev.	
0.0000	1.31260208E+01	1.01451989E-05	A-K
0.0000	1.05637056E+01	4.42235419E-06	A-N
0.0000	9.33726532E-01	4.57193761E-06	a
0.0005	-6.45888382E-04	2.97354219E-07	D-KK
0.0003	-1.42556573E-03	3.77319208E-07	D-KN
0.0001	-9.29004757E-04	1.20339120E-07	D-NN
0.0001	-9.99742362E-04	1.21338538E-07	d-N
0.0000	-1.03513646E-03	4.30702844E-08	d
0.1797	1.18030925E-08	2.12105245E-09	H-KKK
0.0153	-2.76149190E-07	4.22359306E-09	H-KKN
0.0050	6.63636361E-07	3.29508449E-09	H-KNN
5.9416	-4.93907728E-11	7.87369973E-10	H-NNN
0.0259	2.96446972E-08	7.66620478E-10	h-NN
0.0028	1.52323362E-07	4.28933895E-10	h-N
0.0005	1.73719941E-07	8.79181965E-11	h

APPENDIX D

Program used for the solution of the system of equations (VI.1): red.tr.10.

In the results given below, the following data are contained:

non-reduced - S = Transformation from a non-reduced to a S reduced spin-rotor Hamiltonian.
non-reduced - A = Transformation from a non-reduced to an A reduced spin-rotor Hamiltonian.
A - S = Transformation from an A to a S reduced Hamiltonian.
The T's are the parameters in the rotation operator used for the transformation.
The D's are the original Hamiltonian parameters and the D1's are the rotated ones. They correspond to the following operators:

D (1)	D1 (1)	$N \cdot S$
D (2)	D1 (2)	$N_z S_z$
D (3)	D1 (3)	fF
D (4)	D1 (4)	$N^2(N \cdot S)$
D (5)	D1 (5)	$N^2 N_z S_z$
D (6)	D1 (6)	$N^2 fF$
D (7)	D1 (7)	$N_z S_z (N \cdot S)$
D (8)	D1 (8)	$N_z^3 S_z$
D (9)	D1 (9)	$N_z^2 fF$
D (10)	D1 (10)	$f^2(N \cdot S)$
D (11)	D1 (11)	$f^2 N_z S_z$
D (12)	D1 (12)	$f^3 F$
D (13)	D1 (13)	$N^4(N \cdot S)$
D (14)	D1 (14)	$N^4 N_z S_z$
D (15)	D1 (15)	$N^4 fF$
D (16)	D1 (16)	$N^2 N_z^2 (N \cdot S)$
D (17)	D1 (17)	$N^2 N_z^3 S_z$
D (18)	D1 (18)	$N^2 N_z^2 fF$
D (19)	D1 (19)	$N^2 f^2 (N \cdot S)$
D (20)	D1 (20)	$N^2 f^2 N_z S_z$
D (21)	D1 (21)	$N^2 f^3 F$
D (22)	D1 (22)	$N_z^4 (N \cdot S)$
D (23)	D1 (23)	$N_z^5 S_z$
D (24)	D1 (24)	$N_z^4 fF$
D (25)	D1 (25)	$N_z^2 f^2 (N \cdot S)$
D (26)	D1 (26)	$N_z^2 f^2 N_z S_z$
D (27)	D1 (27)	$N_z^2 f^3 F$
D (28)	D1 (28)	$f^4 (N \cdot S)$
D (29)	D1 (29)	$f^4 N_z S_z$
D (30)	D1 (30)	$f^5 F$

ROTATION METHOD FOR A MOLECULE WITH K = -0.5,
AND WITH A TENDENCY = 10^{-2}

nonreduced - S

T(1) = 0.5815115255E-06		
T(2) =-0.1604683336E-05		
T(3) = 0.1789499341E-05		
T(4) = 0.4419957409E-09		
T(5) =-0.2314343679E-08		
T(6) = 0.2098654865E-08		
T(7) = 0.1878429872E-09		
T(8) =-0.2677304565E-08		
T(9) = 0.4738311020E-09		
T(10) =-0.3647638745E-08		
T(11) = 0.2556665428E-08		
T(12) = 0.3504453737E-08		
D(1) =-0.2356707353E-01	D1(1) =-0.2356419926E-01	
D(2) =-0.2790831301E+00	D1(2) =-0.2790931759E+00	
D(3) =-0.9009856223E-02	D1(3) =-0.8989610806E-02	
D(4) = 0.1000000000E-04	D1(4) = 0.8563678762E-05	
D(5) = 0.1000000000E-04	D1(5) =-0.2285511430E-04	
D(6) = 0.1000000000E-06	D1(6) = 0.0	
D(7) = 0.1000000000E-04	D1(7) = 0.8521339510E-04	
D(8) = 0.1000000000E-04	D1(8) = 0.1969383180E-05	
D(9) = 0.1000000000E-06	D1(9) = 0.0	
D(10) = 0.1000000000E-04	D1(10) = 0.1020221482E-04	
D(11) = 0.1000000000E-04	D1(11) = 0.0	
D(12) = 0.1000000000E-06	D1(12) = 0.8170623141E-06	
D(13) = 0.1000000000E-08	D1(13) = 0.2258304686E-08	
D(14) = 0.1000000000E-08	D1(14) =-0.4365109595E-07	
D(15) = 0.1000000000E-10	D1(15) = 0.0	
D(16) = 0.1000000000E-08	D1(16) = 0.9091697631E-07	
D(17) = 0.1000000000E-08	D1(17) =-0.2786873933E-07	
D(18) = 0.1000000000E-10	D1(18) = 0.0	
D(19) = 0.1000000000E-08	D1(19) = 0.9981473464E-09	
D(20) = 0.1000000000E-10	D1(20) = 0.0	
D(21) = 0.1000000000E-10	D1(21) = 0.0	
D(22) = 0.1000000000E-08	D1(22) = 0.3781362701E-07	
D(23) = 0.1000000000E-08	D1(23) = 0.2005076255E-07	
D(24) = 0.1000000000E-10	D1(24) = 0.0	
D(25) = 0.1000000000E-08	D1(25) = 0.0	
D(26) = 0.1000000000E-08	D1(26) = 0.0	
D(27) = 0.1000000000E-10	D1(27) = 0.0	
D(28) = 0.1000000000E-10	D1(28) =-0.5991523432E-09	
D(29) = 0.1000000000E-10	D1(29) = 0.0	
D(30) = 0.1000000000E-10	D1(30) = 0.3185265360E-10	

nonreduced - A

T(1) =-0.9579180975E-07	
T(2) = 0.2096392991E-06	
T(3) =-0.2207358054E-06	
T(4) =-0.2418316704E-10	
T(5) = 0.2407918378E-09	
T(6) =-0.1771471492E-09	

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T( 7) = 0.1724479299E-10
T( 8) = 0.2023642458E-09
T( 9) =-0.1091397367E-09
T(10) = 0.7415129435E-09
T(11) =-0.1282056856E-09
T(12) =-0.7480959296E-09
D( 1) =-0.2356707353E-01      D1( 1) =-0.2356747457E-01
D( 2) =-0.2790831301E+00      D1( 2) =-0.2790817271E+00
D( 3) =-0.9009856223E-02      D1( 3) =-0.9012691677E-02
D( 4) = 0.1000000000E-04      D1( 4) = 0.1020099220E-04
D( 5) = 0.1000000000E-04      D1( 5) = 0.1411757271E-04
D( 6) = 0.1000000000E-06      D1( 6) = 0.0
D( 7) = 0.1000000000E-04      D1( 7) = 0.4449683134E-06
D( 8) = 0.1000000000E-04      D1( 8) = 0.1111623574E-04
D( 9) = 0.1000000000E-06      D1( 9) = 0.0
D(10) = 0.1000000000E-04      D1(10) = 0.1020196000E-04
D(11) = 0.1000000000E-04      D1(11) = 0.1151131062E-04
D(12) = 0.1000000000E-06      D1(12) = 0.0
D(13) = 0.1000000000E-08      D1(13) = 0.6639013610E-09
D(14) = 0.1000000000E-08      D1(14) = 0.4620600934E-08
D(15) = 0.1000000000E-10      D1(15) = 0.0
D(16) = 0.1000000000E-08      D1(16) =-0.4491293792E-08
D(17) = 0.1000000000E-08      D1(17) = 0.1208112481E-07
D(18) = 0.1000000000E-10      D1(18) = 0.0
D(19) = 0.1000000000E-08      D1(19) = 0.1030000000E-08
D(20) = 0.1000000000E-10      D1(20) = 0.0
D(21) = 0.1000000000E-10      D1(21) = 0.9902465975E-10
D(22) = 0.1000000000E-08      D1(22) =-0.2195379694E-07
D(23) = 0.1000000000E-08      D1(23) = 0.3777378966E-09
D(24) = 0.1000000000E-10      D1(24) = 0.0
D(25) = 0.1000000000E-08      D1(25) = 0.0
D(26) = 0.1000000000E-08      D1(26) = 0.3223258416E-08
D(27) = 0.1000000000E-10      D1(27) = 0.0
D(28) = 0.1000000000E-10      D1(28) = 0.0
D(29) = 0.1000000000E-10      D1(29) = 0.0
D(30) = 0.1000000000E-10      D1(30) = 0.0

A - S
T( 1) = 0.6773030154E-06
T( 2) =-0.1814321810E-05
T( 3) = 0.2010234234E-05
T( 4) = 0.4661786688E-09
T( 5) =-0.2555134327E-08
T( 6) = 0.2275800991E-08
T( 7) = 0.1705980889E-09
T( 8) =-0.2879667362E-08
T( 9) = 0.5829706618E-09
T(10) =-0.4389149892E-08
T(11) = 0.2684869772E-08
T(12) = 0.4252547953E-08
D( 1) =-0.2356747457E-01      D1( 1) =-0.2356419925E-01
D( 2) =-0.2790817271E+00      D1( 2) =-0.2790931759E+00
D( 3) =-0.9012691677E-02      D1( 3) =-0.8989610819E-02
D( 4) = 0.1020099220E-04      D1( 4) = 0.8563677604E-05
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D( 5) = 0.1411757271E-04
D( 6) = 0.0
D( 7) = 0.4449683134E-06
D( 8) = 0.1111623574E-04
D( 9) = 0.0
D(10) = 0.1020196000E-04
D(11) = 0.1151131062E-04
D(12) = 0.0
D(13) = 0.6639013610E-09
D(14) = 0.4620600934E-08
D(15) = 0.0
D(16) =-0.4491293792E-08
D(17) = 0.1208112481E-07
D(18) = 0.0
D(19) = 0.1030000000E-08
D(20) = 0.0
D(21) = 0.9902465975E-10
D(22) =-0.2195379694E-07
D(23) = 0.3777378966E-09
D(24) = 0.0
D(25) = 0.0
D(26) = 0.3223258416E-08
D(27) = 0.0
D(28) = 0.0
D(29) = 0.0
D(30) = 0.0
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D1( 5) =-0.2285509683E-04
D1( 6) = 0.0
D1( 7) = 0.8521335471E-04
D1( 8) = 0.1969389754E-05
D1( 9) = 0.0
D1(10) = 0.1020221482E-04
D1(11) = 0.0
D1(12) = 0.8170628942E-06
D1(13) = 0.2258303941E-08
D1(14) =-0.4365107286E-07
D1(15) = 0.0
D1(16) = 0.9091693005E-07
D1(17) =-0.2786872591E-07
D1(18) = 0.0
D1(19) = 0.9981473556E-09
D1(20) = 0.0
D1(21) = 0.0
D1(22) = 0.3781361163E-07
D1(23) = 0.2005075193E-07
D1(24) = 0.0
D1(25) = 0.0
D1(26) = 0.0
D1(27) = 0.0
D1(28) =-0.5991519703E-09
D1(29) = 0.0
D1(30) = 0.3185264438E-10
```

ROTATION METHOD FOR A MOLECULE WITH K = -0.5,
AND WITH A TENDENCY = 10^{-2} IN THE SPIN ROTOR PART

nonreduced - S

```
T( 1) = 0.6264332888E-06
T( 2) =-0.1524537843E-05
T( 3) = 0.1711384601E-05
T( 4) =-0.2795645182E-08
T( 5) = 0.1539405419E-08
T( 6) = 0.1160853972E-08
T( 7) =-0.3322345150E-08
T( 8) = 0.1529221000E-07
T( 9) =-0.8470524039E-09
T(10) =-0.1526714230E-07
T(11) =-0.1229735134E-07
T(12) = 0.1639484437E-07
D( 1) =-0.2356707353E-01
D( 2) =-0.2790831301E+00
D( 3) =-0.9009856223E-02
D( 4) = 0.1000000000E-04
D( 5) = 0.1000000000E-04
D( 6) = 0.1000000000E-06
D( 7) = 0.1000000000E-04
D( 8) = 0.1000000000E-04
D( 9) = 0.1000000000E-06
D(10) = 0.1000000000E-04
```

```
D1( 1) =-0.2356418942E-01
D1( 2) =-0.2790932118E+00
D1( 3) =-0.8989584404E-02
D1( 4) = 0.8557268204E-05
D1( 5) =-0.2235582700E-04
D1( 6) = 0.0
D1( 7) = 0.8420915290E-04
D1( 8) = 0.1981007182E-05
D1( 9) = 0.0
D1(10) = 0.1018946142E-04
```

```
D(11) = 0.1000000000E-04        D1(11) = 0.0
D(12) = 0.1000000000E-06        D1(12) = 0.8195040708E-06
D(13) = 0.1000000000E-08        D1(13) = 0.3021827247E-08
D(14) = 0.1000000000E-08        D1(14) = 0.1298814207E-06
D(15) = 0.1000000000E-10        D1(15) = 0.0
D(16) = 0.1000000000E-08        D1(16) =-0.2618942189E-06
D(17) = 0.1000000000E-08        D1(17) =-0.4617991474E-06
D(18) = 0.1000000000E-10        D1(18) = 0.0
D(19) = 0.1000000000E-08        D1(19) = 0.2592322806E-08
D(20) = 0.1000000000E-10        D1(20) = 0.0
D(21) = 0.1000000000E-10        D1(21) = 0.0
D(22) = 0.1000000000E-08        D1(22) = 0.9133754775E-06
D(23) = 0.1000000000E-08        D1(23) = 0.1733236754E-07
D(24) = 0.1000000000E-10        D1(24) = 0.0
D(25) = 0.1000000000E-08        D1(25) = 0.0
D(26) = 0.1000000000E-08        D1(26) = 0.0
D(27) = 0.1000000000E-10        D1(27) = 0.0
D(28) = 0.1000000000E-10        D1(28) =-0.9809136235E-09
D(29) = 0.1000000000E-10        D1(29) = 0.0
D(30) = 0.1000000000E-10        D1(30) =-0.1562322806E-08

nonreduced - A
T( 1) =-0.9998661497E-07
T( 2) = 0.1788085682E-06
T( 3) =-0.1798518981E-06
T( 4) = 0.3760930838E-09
T( 5) =-0.4978760383E-09
T( 6) =-0.2965412967E-09
T( 7) = 0.9557086580E-09
T( 8) =-0.3410156292E-08
T( 9) =-0.3513823527E-08
T(10) = 0.6576896282E-08
T(11) = 0.2943603292E-08
T(12) =-0.7217541326E-08
D( 1) =-0.2356707353E-01        D1( 1) =-0.2356747420E-01
D( 2) =-0.2790831301E+00        D1( 2) =-0.2790816981E+00
D( 3) =-0.9009856223E-02        D1( 3) =-0.9012905482E-02
D( 4) = 0.1000000000E-04        D1( 4) = 0.1020085653E-04
D( 5) = 0.1000000000E-04        D1( 5) = 0.1380358953E-04
D( 6) = 0.1000000000E-06        D1( 6) = 0.0
D( 7) = 0.1000000000E-04        D1( 7) = 0.9885109964E-06
D( 8) = 0.1000000000E-04        D1( 8) = 0.1128382685E-04
D( 9) = 0.1000000000E-06        D1( 9) = 0.0
D(10) = 0.1000000000E-04        D1(10) = 0.1020196000E-04
D(11) = 0.1000000000E-04        D1(11) = 0.1156454275E-04
D(12) = 0.1000000000E-06        D1(12) = 0.0
D(13) = 0.1000000000E-08        D1(13) = 0.7317325822E-09
D(14) = 0.1000000000E-08        D1(14) =-0.2306921421E-07
D(15) = 0.1000000000E-10        D1(15) = 0.0
D(16) = 0.1000000000E-08        D1(16) = 0.7303388365E-07
D(17) = 0.1000000000E-08        D1(17) = 0.1449067182E-06
D(18) = 0.1000000000E-10        D1(18) = 0.0
D(19) = 0.1000000000E-08        D1(19) = 0.1030000000E-08
D(20) = 0.1000000000E-10        D1(20) = 0.0
```

```
D(21) = 0.1000000000E-10        D1(21) = 0.8206685446E-10
D(22) = 0.1000000000E-08        D1(22) =-0.3624409426E-06
D(23) = 0.1000000000E-08        D1(23) = 0.5300031834E-07
D(24) = 0.1000000000E-10        D1(24) = 0.0
D(25) = 0.1000000000E-08        D1(25) = 0.0
D(26) = 0.1000000000E-08        D1(26) = 0.5625155845E-07
D(27) = 0.1000000000E-10        D1(27) = 0.0
D(28) = 0.1000000000E-10        D1(28) = 0.0
D(29) = 0.1000000000E-10        D1(29) = 0.0
D(30) = 0.1000000000E-10        D1(30) = 0.0

A - S
T( 1) = 0.7264195570E-06
T( 2) =-0.1703345620E-05
T( 3) = 0.1891235619E-05
T( 4) =-0.3171736830E-08
T( 5) = 0.2037280666E-08
T( 6) = 0.1457394723E-08
T( 7) =-0.4278052095E-08
T( 8) = 0.1870235847E-07
T( 9) = 0.2666771627E-08
T(10) =-0.2184403078E-07
T(11) =-0.1524094832E-07
T(12) = 0.2361237732E-07
D( 1) =-0.2356747420E-01        D1( 1) =-0.2356418941E-01
D( 2) =-0.2790816981E+00        D1( 2) =-0.2790932118E+00
D( 3) =-0.9012905482E-02        D1( 3) =-0.8989584418E-02
D( 4) = 0.1020085653E-04        D1( 4) = 0.8557266763E-05
D( 5) = 0.1380358953E-04        D1( 5) =-0.2235580942E-04
D( 6) = 0.0                     D1( 6) = 0.0
D( 7) = 0.9885109964E-06        D1( 7) = 0.8420911310E-04
D( 8) = 0.1128382685E-04        D1( 8) = 0.1981013248E-05
D( 9) = 0.0                     D1( 9) = 0.0
D(10) = 0.1020196000E-04        D1(10) = 0.1018946142E-04
D(11) = 0.1156454275E-04        D1(11) = 0.0
D(12) = 0.0                     D1(12) = 0.8195047926E-06
D(13) = 0.7317325822E-09        D1(13) = 0.3021826086E-08
D(14) =-0.2306921421E-07        D1(14) = 0.1298813545E-06
D(15) = 0.0                     D1(15) = 0.0
D(16) = 0.7303388365E-07        D1(16) =-0.2618940833E-06
D(17) = 0.1449067182E-06        D1(17) =-0.4617989100E-06
D(18) = 0.0                     D1(18) = 0.0
D(19) = 0.1030000000E-08        D1(19) = 0.2592321962E-08
D(20) = 0.0                     D1(20) = 0.0
D(21) = 0.8206685446E-10        D1(21) = 0.0
D(22) =-0.3624409426E-06        D1(22) = 0.9133750101E-06
D(23) = 0.5300031834E-07        D1(23) = 0.1733235827E-07
D(24) = 0.0                     D1(24) = 0.0
D(25) = 0.0                     D1(25) = 0.0
D(26) = 0.5625155845E-07        D1(26) = 0.0
D(27) = 0.0                     D1(27) = 0.0
D(28) = 0.0                     D1(28) =-0.9809130430E-09
D(29) = 0.0                     D1(29) = 0.0
D(30) = 0.0                     D1(30) =-0.1562321962E-08
```

ROTATION METHOD FOR A MOLECULE WITH K = -0.5,
AND WITH A TENDENCY = 10^{-2} IN THE ROTOR PART

nonreduced - S

```
T( 1) =-0.8503235581E-07
T( 2) =-0.4258506975E-05
T( 3) = 0.5866083434E-05
T( 4) = 0.8701202980E-10
T( 5) =-0.6679749599E-08
T( 6) = 0.7289443382E-08
T( 7) = 0.5768902565E-10
T( 8) =-0.5460161950E-08
T( 9) = 0.4199855920E-09
T(10) =-0.1370056555E-07
T(11) = 0.5489510463E-08
T(12) = 0.1401377948E-07
D( 1) =-0.2356707353E-01
D( 2) =-0.2790831301E+00
D( 3) =-0.9009856223E-02
D( 4) = 0.1000000000E-04
D( 5) = 0.1000000000E-04
D( 6) = 0.1000000000E-04
D( 7) = 0.1000000000E-04
D( 8) = 0.1000000000E-04
D( 9) = 0.1000000000E-04
D(10) = 0.1000000000E-04
D(11) = 0.1000000000E-04
D(12) = 0.1000000000E-04
D(13) = 0.1000000000E-08
D(14) = 0.1000000000E-08
D(15) = 0.1000000000E-08
D(16) = 0.1000000000E-08
D(17) = 0.1000000000E-08
D(18) = 0.1000000000E-08
D(19) = 0.1000000000E-08
D(20) = 0.1000000000E-08
D(21) = 0.1000000000E-08
D(22) = 0.1000000000E-08
D(23) = 0.1000000000E-08
D(24) = 0.1000000000E-08
D(25) = 0.1000000000E-08
D(26) = 0.1000000000E-08
D(27) = 0.1000000000E-08
D(28) = 0.1000000000E-08
D(29) = 0.1000000000E-08
D(30) = 0.1000000000E-08
```

```
D1( 1) =-0.2356138691E-01
D1( 2) =-0.2791029825E+00
D1( 3) =-0.8969970372E-02
D1( 4) = 0.7181035490E-05
D1( 5) =-0.9384869263E-04
D1( 6) = 0.0
D1( 7) = 0.2373809156E-03
D1( 8) =-0.6793030326E-05
D1( 9) = 0.0
D1(10) = 0.3000689613E-04
D1(11) = 0.0
D1(12) = 0.1142316975E-04
D1(13) = 0.3312507674E-08
D1(14) =-0.1160098603E-06
D1(15) = 0.0
D1(16) = 0.2375009282E-06
D1(17) =-0.1544086978E-06
D1(18) = 0.0
D1(19) = 0.2887983610E-08
D1(20) = 0.0
D1(21) = 0.0
D1(22) = 0.2688590887E-06
D1(23) = 0.3916459172E-07
D1(24) = 0.0
D1(25) = 0.0
D1(26) = 0.0
D1(27) = 0.0
D1(28) = 0.1843746163E-08
D1(29) = 0.0
D1(30) = 0.1112016390E-08
```

nonreduced -A

```
T( 1) =-0.9576966206E-05
T( 2) = 0.2098902857E-04
T( 3) =-0.2208905548E-04
T( 4) =-0.4024894745E-08
```

```
T( 5) = 0.2567606990E-07
T( 6) =-0.2524612451E-07
T( 7) = 0.8068793092E-09
T( 8) = 0.1953756871E-07
T( 9) =-0.1896230044E-07
T(10) = 0.6953810933E-07
T(11) =-0.1874622743E-07
T(12) =-0.6969339020E-07
D( 1) =-0.2356707353E-01
D( 2) =-0.2790831301E+00
D( 3) =-0.9009856223E-02
D( 4) = 0.1000000000E-04
D( 5) = 0.1000000000E-04
D( 6) = 0.1000000000E-04
D( 7) = 0.1000000000E-04
D( 8) = 0.1000000000E-04
D( 9) = 0.1000000000E-04
D(10) = 0.1000000000E-04
D(11) = 0.1000000000E-04
D(12) = 0.1000000000E-04
D(13) = 0.1000000000E-08
D(14) = 0.1000000000E-08
D(15) = 0.1000000000E-08
D(16) = 0.1000000000E-08
D(17) = 0.1000000000E-08
D(18) = 0.1000000000E-08
D(19) = 0.1000000000E-08
D(20) = 0.1000000000E-08
D(21) = 0.1000000000E-08
D(22) = 0.1000000000E-08
D(23) = 0.1000000000E-08
D(24) = 0.1000000000E-08
D(25) = 0.1000000000E-08
D(26) = 0.1000000000E-08
D(27) = 0.1000000000E-08
D(28) = 0.1000000000E-08
D(29) = 0.1000000000E-08
D(30) = 0.1000000000E-08

D1( 1) =-0.2360717717E-01
D1( 2) =-0.2789428225E+00
D1( 3) =-0.9293399408E-02
D1( 4) = 0.3007097521E-04
D1( 5) = 0.4219540422E-03
D1( 6) = 0.0
D1( 7) =-0.9458098454E-03
D1( 8) = 0.1216361607E-03
D1( 9) = 0.0
D1(10) = 0.2999800000E-04
D1(11) = 0.1611301654E-03
D1(12) = 0.0
D1(13) = 0.1848760406E-07
D1(14) = 0.4315855635E-06
D1(15) = 0.0
D1(16) =-0.7697510608E-06
D1(17) = 0.9366130029E-06
D1(18) = 0.0
D1(19) = 0.4000000000E-08
D1(20) = 0.0
D1(21) = 0.6371901016E-08
D1(22) =-0.1879312165E-05
D1(23) =-0.6084630259E-07
D1(24) = 0.0
D1(25) = 0.0
D1(26) = 0.2233976212E-06
D1(27) = 0.0
D1(28) = 0.0
D1(29) = 0.0
D1(30) = 0.0

A - S
T( 1) = 0.9491488921E-05
T( 2) =-0.2524638767E-04
T( 3) = 0.2795387080E-04
T( 4) = 0.4111574120E-08
T( 5) =-0.3235416518E-07
T( 6) = 0.3253414496E-07
T( 7) =-0.7493367750E-09
T( 8) =-0.2499571620E-07
T( 9) = 0.1938203987E-07
T(10) =-0.8323617608E-07
T(11) = 0.2423387187E-07
T(12) = 0.8370478737E-07
D( 1) =-0.2360717717E-01
D( 2) =-0.2789428225E+00

D1( 1) =-0.2356138058E-01
D1( 2) =-0.2791030032E+00
```

```
D( 3) =-0.9293399408E-02
D( 4) = 0.3007097521E-04
D( 5) = 0.4219540422E-03
D( 6) = 0.0
D( 7) =-0.9458098454E-03
D( 8) = 0.1216361607E-03
D( 9) = 0.0
D(10) = 0.2999800000E-04
D(11) = 0.1611301654E-03
D(12) = 0.0
D(13) =-0.1848760406E-07
D(14) = 0.4315855635E-06
D(15) = 0.0
D(16) =-0.7697510608E-06
D(17) = 0.9366130029E-06
D(18) = 0.0
D(19) = 0.4000000000E-08
D(20) = 0.0
D(21) = 0.6371901016E-08
D(22) =-0.1879312165E-05
D(23) =-0.6084630259E-07
D(24) = 0.0
D(25) = 0.0
D(26) = 0.2233976212E-06
D(27) = 0.0
D(28) = 0.0
D(29) = 0.0
D(30) = 0.0
```

```
D1( 3) =-0.8969989616E-02
D1( 4) = 0.7179404016E-05
D1( 5) =-0.9382438248E-04
D1( 6) = 0.0
D1( 7) = 0.2373247645E-03
D1( 8) =-0.6783896442E-05
D1( 9) = 0.0
D1(10) = 0.3000689603E-04
D1(11) = 0.0
D1(12) = 0.1142398652E-04
D1(13) = 0.3311470160E-08
D1(14) =-0.1159777472E-06
D1(15) = 0.0
D1(16) = 0.2374365936E-06
D1(17) =-0.1543900459E-06
D1(18) = 0.0
D1(19) = 0.2887996425E-08
D1(20) = 0.0
D1(21) = 0.0
D1(22) = 0.2688377089E-06
D1(23) = 0.3914981365E-07
D1(24) = 0.0
D1(25) = 0.0
D1(26) = 0.0
D1(27) = 0.0
D1(28) = 0.1844264920E-08
D1(29) = 0.0
D1(30) = 0.1112003575E-08
```

ROTATION METHOD FOR A MOLECULE WITH K = -0.5,
WITHOUT A TENDENCY

nonreduced - S

```
T( 1) = 0.4716282872E-07
T( 2) =-0.4020321286E-05
T( 3) = 0.5633771045E-05
T( 4) =-0.9196369655E-08
T( 5) = 0.5076353939E-08
T( 6) = 0.4167427602E-08
T( 7) =-0.9952523694E-08
T( 8) = 0.4849779475E-07
T( 9) =-0.3517323924E-08
T(10) =-0.4886783774E-07
T(11) =-0.3926428511E-07
T(12) = 0.5302595615E-07
D( 1) =-0.2356707353E-01
D( 2) =-0.2790831301E+00
D( 3) =-0.9009856223E-02
D( 4) = 0.1000000000E-04
D( 5) = 0.1000000000E-04
D( 6) = 0.1000000000E-04
D( 7) = 0.1000000000E-04
D( 8) = 0.1000000000E-04
```

```
D1( 1) =-0.2356136651E-01
D1( 2) =-0.2791030564E+00
D1( 3) =-0.8969909880E-02
D1( 4) = 0.7167667722E-05
D1( 5) =-0.9241774139E-04
D1( 6) = 0.0
D1( 7) =-0.2344639653E-03
D1( 8) =-0.6723420933E-05
```

```
D( 9) = 0.1000000000E-04
D(10) = 0.1000000000E-04
D(11) = 0.1000000000E-04
D(12) = 0.1000000000E-04
D(13) = 0.1000000000E-08
D(14) = 0.1000000000E-08
D(15) = 0.1000000000E-08
D(16) = 0.1000000000E-08
D(17) = 0.1000000000E-08
D(18) = 0.1000000000E-08
D(19) = 0.1000000000E-08
D(20) = 0.1000000000E-08
D(21) = 0.1000000000E-08
D(22) = 0.1000000000E-08
D(23) = 0.1000000000E-08
D(24) = 0.1000000000E-08
D(25) = 0.1000000000E-08
D(26) = 0.1000000000E-08
D(27) = 0.1000000000E-08
D(28) = 0.1000000000E-08
D(29) = 0.1000000000E-08
D(30) = 0.1000000000E-08
```

```
D1( 9) = 0.0
D1(10) = 0.2998086299E-04
D1(11) = 0.0
D1(12) = 0.1142821715E-04
D1(13) = 0.4948985104E-08
D1(14) = 0.4114319875E-06
D1(15) = 0.0
D1(16) =-0.8291075946E-06
D1(17) =-0.1471810960E-05
D1(18) = 0.0
D1(19) = 0.6142126774E-08
D1(20) = 0.0
D1(21) = 0.0
D1(22) = 0.2918199210E-05
D1(23) = 0.3471734567E-07
D1(24) = 0.0
D1(25) = 0.0
D1(26) = 0.0
D1(27) = 0.0
D1(28) = 0.1025507448E-08
D1(29) = 0.0
D1(30) =-0.2142126774E-08
```

nonreduced - A

```
T( 1) =-0.9997106842E-05
T( 2) = 0.1790696962E-04
T( 3) =-0.1800273990E-04
T( 4) = 0.3603956506E-07
T( 5) =-0.4819849222E-07
T( 6) =-0.3716889423E-07
T( 7) = 0.9464133519E-07
T( 8) =-0.3417872909E-06
T( 9) =-0.3590577577E-06
T(10) = 0.6527817036E-06
T(11) = 0.2884795337E-06
T(12) =-0.7163113983E-06
D( 1) =-0.2356707353E-01
D( 2) =-0.2790831301E+00
D( 3) =-0.9009856223E-02
D( 4) = 0.1000000000E-04
D( 5) = 0.1000000000E-04
D( 6) = 0.1000000000E-04
D( 7) = 0.1000000000E-04
D( 8) = 0.1000000000E-04
D( 9) = 0.1000000000E-04
D(10) = 0.1000000000E-04
D(11) = 0.1000000000E-04
D(12) = 0.1000000000E-04
D(13) = 0.1000000000E-08
D(14) = 0.1000000000E-08
D(15) = 0.1000000000E-08
D(16) = 0.1000000000E-08
D(17) = 0.1000000000E-08
D(18) = 0.1000000000E-08
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D1( 1) =-0.2360714098E-01
D1( 2) =-0.2789399272E+00
D1( 3) =-0.9314758612E-02
D1( 4) = 0.3005742675E-04
D1( 5) = 0.3905733220E-03
D1( 6) = 0.0
D1( 7) =-0.8914810787E-03
D1( 8) = 0.1383771785E-03
D1( 9) = 0.0
D1(10) = 0.2999800000E-04
D1(11) = 0.1664480168E-03
D1(12) = 0.0
D1(13) =-0.1171337558E-07
D1(14) =-0.2338649345E-05
D1(15) = 0.0
D1(16) = 0.6983052770E-05
D1(17) = 0.1421644074E-04
D1(18) = 0.0
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D(19) = 0.1000000000E-08        D1(19) = 0.4000000000E-08
D(20) = 0.1000000000E-08        D1(20) = 0.0
D(21) = 0.1000000000E-08        D1(21) = 0.4678343896E-08
D(22) = 0.1000000000E-08        D1(22) =-0.3591502777E-04
D(23) = 0.1000000000E-08        D1(23) = 0.5196105595E-05
D(24) = 0.1000000000E-08        D1(24) = 0.0
D(25) = 0.1000000000E-08        D1(25) = 0.0
D(26) = 0.1000000000E-08        D1(26) = 0.5520910375E-05
D(27) = 0.1000000000E-08        D1(27) = 0.0
D(28) = 0.1000000000E-08        D1(28) = 0.0
D(29) = 0.1000000000E-08        D1(29) = 0.0
D(30) = 0.1000000000E-08        D1(30) = 0.0

A - S
T( 1) = 0.1004382919E-04
T( 2) =-0.2192628963E-04
T( 3) = 0.2363539694E-04
T( 4) =-0.4523411813E-07
T( 5) = 0.5327384378E-07
T( 6) = 0.4133563304E-07
T( 7) =-0.1045916901E-06
T( 8) = 0.3902751935E-06
T( 9) = 0.3555410708E-06
T(10) =-0.7016396637E-06
T(11) =-0.3277358251E-06
T(12) = 0.7693267542E-06
D( 1) =-0.2360714098E-01        D1( 1) =-0.2356136027E-01
D( 2) =-0.2789399272E+00        D1( 2) =-0.2791030772E+00
D( 3) =-0.9314758612E-02        D1( 3) =-0.8969928125E-02
D( 4) = 0.3005742675E-04        D1( 4) = 0.7165589410E-05
D( 5) = 0.3905733220E-03        D1( 5) =-0.9239557953E-04
D( 6) = 0.0                     D1( 6) = 0.0
D( 7) =-0.8914810787E-03        D1( 7) = 0.2344138340E-03
D( 8) = 0.1383771785E-03        D1( 8) =-0.6715560936E-05
D( 9) = 0.0                     D1( 9) = 0.0
D(10) = 0.2999800000E-04        D1(10) = 0.2998087157E-04
D(11) = 0.1664480168E-03        D1(11) = 0.0
D(12) = 0.0                     D1(12) = 0.1142925779E-04
D(13) =-0.1171337558E-07        D1(13) = 0.4947508818E-08
D(14) =-0.2338649345E-05        D1(14) = 0.4113480948E-06
D(15) = 0.0                     D1(15) = 0.0
D(16) = 0.6983052770E-05        D1(16) =-0.8289360004E-06
D(17) = 0.1421644074E-04        D1(17) =-0.1471510524E-05
D(18) = 0.0                     D1(18) = 0.0
D(19) = 0.4000000000E-08        D1(19) = 0.6141054196E-08
D(20) = 0.0                     D1(20) = 0.0
D(21) = 0.4678343896E-08        D1(21) = 0.0
D(22) =-0.3591502777E-04        D1(22) = 0.2917607785E-05
D(23) = 0.5196105595E-05        D1(23) = 0.3470556469E-07
D(24) = 0.0                     D1(24) = 0.0
D(25) = 0.0                     D1(25) = 0.0
D(26) = 0.5520910375E-05        D1(26) = 0.0
D(27) = 0.0                     D1(27) = 0.0
D(28) = 0.0                     D1(28) = 0.1026245591E-08
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D(29) = 0.0                          D1(29) = 0.0
D(30) = 0.0                          D1(30) =-0.2141054196E-08


ROTATION METHOD FOR A MOLECULE WITH K = -0.9,
AND WITH A TENDENCY = 10⁻²

nonreduced - S
T( 1) = 0.5797294721E-06
T( 2) =-0.9013040386E-05
T( 3) = 0.9262303187E-05
T( 4) = 0.9166590071E-09
T( 5) =-0.6550197278E-07
T( 6) = 0.6479320552E-07
T( 7) = 0.6619411139E-09
T( 8) =-0.6521483138E-07
T( 9) = 0.1044292718E-08
T(10) =-0.1215511588E-06
T(11) = 0.6462355606E-07
T(12) = 0.1208505907E-06
D( 1) =-0.2356707353E-01          D1( 1) =-0.2356656701E-01
D( 2) =-0.2790831301E+00          D1( 2) =-0.2790848891E+00
D( 3) =-0.1621607474E-02          D1( 3) =-0.1601355408E-02
D( 4) = 0.1000000000E-04          D1( 4) = 0.9744329944E-05
D( 5) = 0.1000000000E-04          D1( 5) =-0.1897058080E-03
D( 6) = 0.1000000000E-06          D1( 6) = 0.0
D( 7) = 0.1000000000E-04          D1( 7) = 0.4159895083E-03
D( 8) = 0.1000000000E-04          D1( 8) = 0.3721552385E-05
D( 9) = 0.1000000000E-06          D1( 9) = 0.0
D(10) = 0.1000000000E-04          D1(10) = 0.1020195353E-04
D(11) = 0.1000000000E-04          D1(11) = 0.0
D(12) = 0.1000000000E-06          D1(12) = 0.2263839043E-06
D(13) = 0.1000000000E-08          D1(13) = 0.2611123474E-08
D(14) = 0.1000000000E-08          D1(14) =-0.1338129669E-05
D(15) = 0.1000000000E-10          D1(15) = 0.0
D(16) = 0.1000000000E-08          D1(16) = 0.2679334143E-05
D(17) = 0.1000000000E-08          D1(17) =-0.1175371896E-05
D(18) = 0.1000000000E-10          D1(18) = 0.0
D(19) = 0.1000000000E-08          D1(19) = 0.1030808547E-08
D(20) = 0.1000000000E-10          D1(20) = 0.0
D(21) = 0.1000000000E-10          D1(21) = 0.0
D(22) = 0.1000000000E-08          D1(22) = 0.2329327587E-05
D(23) = 0.1000000000E-08          D1(23) = 0.2373027534E-07
D(24) = 0.1000000000E-10          D1(24) = 0.0
D(25) = 0.1000000000E-08          D1(25) = 0.0
D(26) = 0.1000000000E-08          D1(26) = 0.0
D(27) = 0.1000000000E-10          D1(27) = 0.0
D(28) = 0.1000000000E-10          D1(28) =-0.7755617370E-09
D(29) = 0.1000000000E-10          D1(29) = 0.0
D(30) = 0.1000000000E-10          D1(30) =-0.8085466975E-12

nonreduced - A
T( 1) =-0.4876298211E-06
T( 2) = 0.6562747416E-05
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T( 3) =-0.6687420976E-05
T( 4) = 0.6909127537E-09
T( 5) = 0.2679069465E-07
T( 6) =-0.2772069725E-07
T( 7) = 0.1095363177E-08
T( 8) = 0.2019224047E-07
T( 9) =-0.1032526379E-07
T(10) = 0.1739659363E-06
T(11) =-0.2099774188E-07
T(12) =-0.1750247677E-06
D( 1) =-0.2356707353E-01      D1( 1) =-0.2356747497E-01
D( 2) =-0.2790831301E+00      D1( 2) =-0.2790817199E+00
D( 3) =-0.1621607474E-02      D1( 3) =-0.1638232248E-02
D( 4) = 0.1000000000E-04      D1( 4) = 0.1020278630E-04
D( 5) = 0.1000000000E-04      D1( 5) = 0.1606323946E-03
D( 6) = 0.1000000000E-06      D1( 6) = 0.0
D( 7) = 0.1000000000E-04      D1( 7) =-0.2961899350E-03
D( 8) = 0.1000000000E-04      D1( 8) = 0.1473147899E-04
D( 9) = 0.1000000000E-06      D1( 9) = 0.0
D(10) = 0.1000000000E-04      D1(10) = 0.1020196000E-04
D(11) = 0.1000000000E-04      D1(11) = 0.1824106398E-04
D(12) = 0.1000000000E-06      D1(12) = 0.0
D(13) = 0.1000000000E-08      D1(13) =-0.2331480036E-09
D(14) = 0.1000000000E-08      D1(14) = 0.4858525927E-06
D(15) = 0.1000000000E-10      D1(15) = 0.0
D(16) = 0.1000000000E-08      D1(16) =-0.9571375989E-06
D(17) = 0.1000000000E-08      D1(17) = 0.3157824230E-05
D(18) = 0.1000000000E-10      D1(18) = 0.0
D(19) = 0.1000000000E-08      D1(19) = 0.1030000000E-08
D(20) = 0.1000000000E-10      D1(20) = 0.0
D(21) = 0.1000000000E-10      D1(21) = 0.3232870009E-09
D(22) = 0.1000000000E-08      D1(22) =-0.6332709862E-05
D(23) = 0.1000000000E-08      D1(23) = 0.1072696302E-07
D(24) = 0.1000000000E-10      D1(24) = 0.0
D(25) = 0.1000000000E-08      D1(25) = 0.0
D(26) = 0.1000000000E-08      D1(26) = 0.1496105010E-06
D(27) = 0.1000000000E-10      D1(27) = 0.0
D(28) = 0.1000000000E-10      D1(28) = 0.0
D(29) = 0.1000000000E-10      D1(29) = 0.0
D(30) = 0.1000000000E-10      D1(30) = 0.0

A - S
T( 1) = 0.1067343936E-05
T( 2) =-0.1557555633E-04
T( 3) = 0.1594948656E-04
T( 4) = 0.2257214771E-09
T( 5) =-0.9229097166E-07
T( 6) = 0.9251222848E-07
T( 7) =-0.4334401678E-09
T( 8) =-0.8540537657E-07
T( 9) = 0.1136953286E-07
T(10) =-0.2955140104E-06
T(11) = 0.8561962087E-07
T(12) = 0.2958722925E-06
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D(1) =-0.2356747497E-01	D1(1) =-0.2356656697E-01
D(2) =-0.2790817199E+00	D1(2) =-0.2790848893E+00
D(3) =-0.1638232248E-02	D1(3) =-0.1601355958E-02
D(4) = 0.1020278630E-04	D1(4) = 0.9744318833E-05
D(5) = 0.1606323946E-03	D1(5) =-0.1897006762E-03
D(6) = 0.0	D1(6) = 0.0
D(7) =-0.2961899350E-03	D1(7) = 0.4159790790E-03
D(8) = 0.1473147899E-04	D1(8) = 0.3721728118E-05
D(9) = 0.0	D1(9) = 0.0
D(10) = 0.1020196000E-04	D1(10) = 0.1020195353E-04
D(11) = 0.1824106398E-04	D1(11) = 0.0
D(12) = 0.0	D1(12) = 0.2263895022E-06
D(13) =-0.2331480036E-09	D1(13) = 0.2611081037E-08
D(14) = 0.4858525927E-06	D1(14) =-0.1338094953E-05
D(15) = 0.0	D1(15) = 0.0
D(16) =-0.9571375989E-06	D1(16) = 0.2679264712E-05
D(17) = 0.3157824230E-05	D1(17) =-0.1175342791E-05
D(18) = 0.0	D1(18) = 0.0
D(19) = 0.1030000000E-08	D1(19) = 0.1030808260E-08
D(20) = 0.0	D1(20) = 0.0
D(21) = 0.3232870009E-09	D1(21) = 0.0
D(22) =-0.6332709862E-05	D1(22) = 0.2329270014E-05
D(23) = 0.1072696302E-07	D1(23) = 0.2372968150E-07
D(24) = 0.0	D1(24) = 0.0
D(25) = 0.0	D1(25) = 0.0
D(26) = 0.1496105010E-06	D1(26) = 0.0
D(27) = 0.0	D1(27) = 0.0
D(28) = 0.0	D1(28) =-0.7755405184E-09
D(29) = 0.0	D1(29) = 0.0
D(30) = 0.0	D1(30) =-0.8082600064E-12

ROTATION METHOD FOR A MOLECULE WITH K = -0.9,
AND WITH A TENDENCY = 10^{-2} IN THE SPIN ROTOR-PART

nonreduced - S

T(1) = 0.1191451759E-05	
T(2) =-0.4260087460E-05	
T(3) = 0.3940824717E-05	
T(4) =-0.4343195740E-07	
T(5) = 0.5867952173E-06	
T(6) =-0.5435369350E-06	
T(7) =-0.4438259001E-07	
T(8) = 0.7847114341E-06	
T(9) =-0.1716021119E-07	
T(10) =-0.1023161329E-05	
T(11) =-0.7406592232E-06	
T(12) = 0.1040609351E-05	
D(1) =-0.2356707353E-01	D1(1) =-0.2356656509E-01
D(2) =-0.2790831301E+00	D1(2) =-0.2790848975E+00
D(3) =-0.1621607474E-02	D1(3) =-0.1601233057E-02
D(4) = 0.1000000000E-04	D1(4) = 0.9741087380E-05
D(5) = 0.1000000000E-04	D1(5) =-0.1536565491E-03
D(6) = 0.1000000000E-06	D1(6) = 0.0

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D( 7) = 0.1000000000E-04        D1( 7) = 0.3410911008E-03
D( 8) = 0.1000000000E-04        D1( 8) = 0.6526434221E-05
D( 9) = 0.1000000000E-06        D1( 9) = 0.0
D(10) = 0.1000000000E-04        D1(10) = 0.1018813770E-04
D(11) = 0.1000000000E-04        D1(11) = 0.0
D(12) = 0.1000000000E-06        D1(12) = 0.2277871363E-06
D(13) = 0.1000000000E-08        D1(13) = 0.2829173884E-08
D(14) = 0.1000000000E-08        D1(14) = 0.1398547551E-04
D(15) = 0.1000000000E-10        D1(15) = 0.0
D(16) = 0.1000000000E-08        D1(16) =-0.2796900469E-04
D(17) = 0.1000000000E-08        D1(17) =-0.3577958084E-04
D(18) = 0.1000000000E-10        D1(18) = 0.0
D(19) = 0.1000000000E-08        D1(19) = 0.2757787547E-08
D(20) = 0.1000000000E-10        D1(20) = 0.0
D(21) = 0.1000000000E-10        D1(21) = 0.0
D(22) = 0.1000000000E-08        D1(22) = 0.7153823630E-04
D(23) = 0.1000000000E-08        D1(23) = 0.2414987321E-07
D(24) = 0.1000000000E-10        D1(24) = 0.0
D(25) = 0.1000000000E-08        D1(25) = 0.0
D(26) = 0.1000000000E-08        D1(26) = 0.0
D(27) = 0.1000000000E-10        D1(27) = 0.0
D(28) = 0.1000000000E-10        D1(28) =-0.8845869421E-09
D(29) = 0.1000000000E-10        D1(29) = 0.0
D(30) = 0.1000000000E-10        D1(30) =-0.1727787547E-08

nonreduced - A
T( 1) =-0.5978534327E-06
T( 2) = 0.1223325657E-05
T( 3) =-0.7347397551E-06
T( 4) = 0.2021185551E-07
T( 5) =-0.2996354869E-06
T( 6) = 0.2767389348E-06
T( 7) = 0.2377118725E-07
T( 8) =-0.3976383105E-06
T( 9) =-0.1198685618E-06
T(10) = 0.1166224830E-05
T(11) = 0.3766163753E-06
T(12) =-0.1187293675E-05
D( 1) =-0.2356707353E-01        D1( 1) =-0.2356747100E-01
D( 2) =-0.2790831301E+00        D1( 2) =-0.2790815494E+00
D( 3) =-0.1621607474E-02        D1( 3) =-0.1644650542E-02
D( 4) = 0.1000000000E-04        D1( 4) = 0.1020077879E-04
D( 5) = 0.1000000000E-04        D1( 5) = 0.1107491586E-03
D( 6) = 0.1000000000E-06        D1( 6) = 0.0
D( 7) = 0.1000000000E-04        D1( 7) =-0.1939007443E-03
D( 8) = 0.1000000000E-04        D1( 8) = 0.1271742346E-04
D( 9) = 0.1000000000E-06        D1( 9) = 0.0
D(10) = 0.1000000000E-04        D1(10) = 0.1020196000E-04
D(11) = 0.1000000000E-04        D1(11) = 0.1973099056E-04
D(12) = 0.1000000000E-06        D1(12) = 0.0
D(13) = 0.1000000000E-08        D1(13) = 0.7706049366E-09
D(14) = 0.1000000000E-08        D1(14) =-0.7071350068E-05
D(15) = 0.1000000000E-10        D1(15) = 0.0
D(16) = 0.1000000000E-08        D1(16) = 0.1428805526E-04
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D(17) = 0.1000000000E-08        D1(17) = 0.3177521816E-04
D(18) = 0.1000000000E-10        D1(18) = 0.0
D(19) = 0.1000000000E-08        D1(19) = 0.1030000000E-08
D(20) = 0.1000000000E-10        D1(20) = 0.0
D(21) = 0.1000000000E-10        D1(21) = 0.7234876586E-10
D(22) = 0.1000000000E-08        D1(22) =-0.6401851247E-04
D(23) = 0.1000000000E-08        D1(23) = 0.3299504276E-06
D(24) = 0.1000000000E-10        D1(24) = 0.0
D(25) = 0.1000000000E-08        D1(25) = 0.0
D(26) = 0.1000000000E-08        D1(26) = 0.185157694 1E-05
D(27) = 0.1000000000E-10        D1(27) = 0.0
D(28) = 0.1000000000E-10        D1(28) = 0.0
D(29) = 0.1000000000E-10        D1(29) = 0.0
D(30) = 0.1000000000E-10        D1(30) = 0.0

A - S
T( 1) = 0.1789291312E-05
T( 2) =-0.5483364284E-05
T( 3) = 0.4675519398E-05
T( 4) =-0.6364331613E-07
T( 5) = 0.8864239920E-06
T( 6) =-0.8202696514E-06
T( 7) =-0.6815326952E-07
T( 8) = 0.1182340769E-05
T( 9) = 0.1027085485E-06
T(10) =-0.2189374460E-05
T(11) =-0.1117267126E-05
T(12) = 0.2227891128E-05
D( 1) =-0.2356747100E-01        D1( 1) =-0.2356656509E-01
D( 2) =-0.2790815494E+00        D1( 2) =-0.2790848975E+00
D( 3) =-0.1644650542E-02        D1( 3) =-0.1601233317E-02
D( 4) = 0.1020077879E-04        D1( 4) = 0.9741049159E-05
D( 5) = 0.1107491586E-03        D1( 5) =-0.1536546765E-03
D( 6) = 0.0                     D1( 6) = 0.0
D( 7) =-0.1939007443E-03        D1( 7) = 0.3410873413E-03
D( 8) = 0.1271742346E-04        D1( 8) = 0.6526486251E-05
D( 9) = 0.0                     D1( 9) = 0.0
D(10) = 0.1020196000E-04        D1(10) = 0.1018813786E-04
D(11) = 0.1973099056E-04        D1(11) = 0.0
D(12) = 0.0                     D1(12) = 0.2278062684E-06
D(13) = 0.7706049366E-09        D1(13) = 0.2829152356E-08
D(14) =-0.7071350068E-05        D1(14) = 0.1398531555E-04
D(15) = 0.0                     D1(15) = 0.0
D(16) = 0.1428805526E-04        D1(16) =-0.2796868475E-04
D(17) = 0.3177521816E-04        D1(17) =-0.3577917165E-04
D(18) = 0.0                     D1(18) = 0.0
D(19) = 0.1030000000E-08        D1(19) = 0.2757767380E-08
D(20) = 0.0                     D1(20) = 0.0
D(21) = 0.7234876586E-10        D1(21) = 0.0
D(22) =-0.6401851247E-04        D1(22) = 0.7153741820E-04
D(23) = 0.3299504276E-06        D1(23) = 0.2414960250E-07
D(24) = 0.0                     D1(24) = 0.0
D(25) = 0.0                     D1(25) = 0.0
D(26) = 0.1851576941E-05        D1(26) = 0.0
```

```
D(27) = 0.0                    D1(27) = 0.0
D(28) = 0.0                    D1(28) =-0.8845761782E-09
D(29) = 0.0                    D1(29) = 0.0
D(30) = 0.0                    D1(30) =-0.1727767380E-08
```

ROTATION METHOD FOR A MOLECULE WITH K = -0.9,
AND WITH A TENDENCY = 10^{-2} IN THE ROTOR PART

nonreduced - S

```
T( 1) =-0.4968191917E-07
T( 2) =-0.2605628777E-04
T( 3) = 0.2781409485E-04
T( 4) =-0.1418028447E-08
T( 5) =-0.1475181536E-06
T( 6) = 0.1495867882E-06
T( 7) =-0.1505960476E-08
T( 8) =-0.1311847267E-06
T( 9) = 0.9033770338E-09
T(10) =-0.4407307430E-06
T(11) = 0.1327604743E-06
T(12) = 0.4405983443E-06
D( 1) =-0.2356707353E-01       D1( 1) =-0.2356607214E-01
D( 2) =-0.2790831301E+00       D1( 2) =-0.2790866025E+00
D( 3) =-0.1621607474E-02       D1( 3) =-0.1581700417E-02
D( 4) = 0.1000000000E-04       D1( 4) = 0.9498417779E-05
D( 5) = 0.1000000000E-04       D1( 5) =-0.5858721782E-03
D( 6) = 0.1000000000E-04       D1( 6) = 0.0
D( 7) = 0.1000000000E-04       D1( 7) = 0.1219683993E-02
D( 8) = 0.1000000000E-04       D1( 8) =-0.7347941434E-05
D( 9) = 0.1000000000E-04       D1( 9) = 0.0
D(10) = 0.1000000000E-04       D1(10) = 0.3000592212E-04
D(11) = 0.1000000000E-04       D1(11) = 0.0
D(12) = 0.1000000000E-04       D1(12) = 0.1026349605E-04
D(13) = 0.1000000000E-08       D1(13) = 0.4295060306E-08
D(14) = 0.1000000000E-08       D1(14) =-0.2864256717E-05
D(15) = 0.1000000000E-08       D1(15) = 0.0
D(16) = 0.1000000000E-08       D1(16) = 0.5731825946E-05
D(17) = 0.1000000000E-08       D1(17) =-0.6295191855E-05
D(18) = 0.1000000000E-08       D1(18) = 0.0
D(19) = 0.1000000000E-08       D1(19) = 0.3009735051E-08
D(20) = 0.1000000000E-08       D1(20) = 0.0
D(21) = 0.1000000000E-08       D1(21) = 0.0
D(22) = 0.1000000000E-08       D1(22) = 0.1254291610E-04
D(23) = 0.1000000000E-08       D1(23) = 0.4786003684E-07
D(24) = 0.1000000000E-08       D1(24) = 0.0
D(25) = 0.1000000000E-08       D1(25) = 0.0
D(26) = 0.1000000000E-08       D1(26) = 0.0
D(27) = 0.1000000000E-08       D1(27) = 0.0
D(28) = 0.1000000000E-08       D1(28) = 0.1352469847E-08
D(29) = 0.1000000000E-08       D1(29) = 0.0
D(30) = 0.1000000000E-08       D1(30) = 0.9902649494E-09
```

nonreduced - A

```
T( 1) =-0.4876114932E-04
T( 2) = 0.6564022170E-03
T( 3) =-0.6688775093E-03
T( 4) = 0.6778935662E-07
T( 5) = 0.2697210042E-05
T( 6) =-0.2796452865E-05
T( 7) = 0.1083592578E-06
T( 8) = 0.2035270118E-05
T( 9) =-0.1040624935E-05
T(10) = 0.1737149731E-04
T(11) =-0.2122184777E-05
T(12) =-0.1747687623E-04
D( 1) =-0.2356707353E-01      D1( 1) =-0.2360721845E-01
D( 2) =-0.2790831301E+00      D1( 2) =-0.2789421076E+00
D( 3) =-0.1621607474E-02      D1( 3) =-0.3284092367E-02
D( 4) = 0.1000000000E-04      D1( 4) = 0.3027357823E-04
D( 5) = 0.1000000000E-04      D1( 5) = 0.1507429638E-01
D( 6) = 0.1000000000E-04      D1( 6) = 0.0
D( 7) = 0.1000000000E-04      D1( 7) =-0.3061116296E-01
D( 8) = 0.1000000000E-04      D1( 8) = 0.4832211251E-03
D( 9) = 0.1000000000E-04      D1( 9) = 0.0
D(10) = 0.1000000000E-04      D1(10) = 0.2999800000E-04
D(11) = 0.1000000000E-04      D1(11) = 0.8341098237E-03
D(12) = 0.1000000000E-04      D1(12) = 0.0
D(13) = 0.1000000000E-08      D1(13) =-0.1197891154E-06
D(14) = 0.1000000000E-08      D1(14) = 0.4891224343E-04
D(15) = 0.1000000000E-08      D1(15) = 0.0
D(16) = 0.1000000000E-08      D1(16) =-0.9667990378E-04
D(17) = 0.1000000000E-08      D1(17) = 0.3147209043E-03
D(18) = 0.1000000000E-08      D1(18) = 0.0
D(19) = 0.1000000000E-08      D1(19) = 0.4000000000E-08
D(20) = 0.1000000000E-08      D1(20) = 0.0
D(21) = 0.1000000000E-08      D1(21) = 0.3169727884E-07
D(22) = 0.1000000000E-08      D1(22) =-0.6314322488E-03
D(23) = 0.1000000000E-08      D1(23) = 0.9736462234E-06
D(24) = 0.1000000000E-08      D1(24) = 0.0
D(25) = 0.1000000000E-08      D1(25) = 0.0
D(26) = 0.1000000000E-08      D1(26) = 0.1486271146E-04
D(27) = 0.1000000000E-08      D1(27) = 0.0
D(28) = 0.1000000000E-08      D1(28) = 0.0
D(29) = 0.1000000000E-08      D1(29) = 0.0
D(30) = 0.1000000000E-08      D1(30) = 0.0

A - S
T( 1) = 0.4864438152E-04
T( 2) =-0.6814473717E-03
T( 3) = 0.6956536910E-03
T( 4) =-0.6931562312E-07
T( 5) =-0.2837320525E-05
T( 6) = 0.2938725831E-05
T( 7) =-0.1099443100E-06
T( 8) =-0.2159049297E-05
T( 9) = 0.1041425045E-05
T(10) =-0.1779875360E-04
```

```
T(11) = 0.2247619264E-05
T(12) = 0.1790408198E-04
D( 1) =-0.2360721845E-01
D( 2) =-0.2789421076E+00
D( 3) =-0.3284092367E-02
D( 4) = 0.3027357823E-04
D( 5) = 0.1507429638E-01
D( 6) = 0.0
D( 7) =-0.3061116296E-01
D( 8) = 0.4832211251E-03
D( 9) = 0.0
D(10) = 0.2999800000E-04
D(11) = 0.8341098237E-03
D(12) = 0.0
D(13) =-0.1197891154E-06
D(14) = 0.4891224343E-04
D(15) = 0.0
D(16) =-0.9667990378E-04
D(17) = 0.3147209043E-03
D(18) = 0.0
D(19) = 0.4000000000E-08
D(20) = 0.0
D(21) = 0.3169727884E-07
D(22) =-0.6314322488E-03
D(23) = 0.9736462234E-06
D(24) = 0.0
D(25) = 0.0
D(26) = 0.1486271146E-04
D(27) = 0.0
D(28) = 0.0
D(29) = 0.0
D(30) = 0.0

D1( 1) =-0.2356587332E-01
D1( 2) =-0.2790872527E+00
D1( 3) =-0.1584103646E-02
D1( 4) = 0.9446525641E-05
D1( 5) =-0.5634571930E-03
D1( 6) = 0.0
D1( 7) = 0.1174129535E-02
D1( 8) =-0.6576566232E-05
D1( 9) = 0.0
D1(10) = 0.3000593214E-04
D1(11) = 0.0
D1(12) = 0.1028962751E-04
D1(13) = 0.4109670359E-08
D1(14) =-0.2712606946E-05
D1(15) = 0.0
D1(16) = 0.5428526934E-05
D1(17) =-0.6168060703E-05
D1(18) = 0.0
D1(19) = 0.3008482624E-08
D1(20) = 0.0
D1(21) = 0.0
D1(22) = 0.1229143288E-04
D1(23) = 0.4526581502E-07
D1(24) = 0.0
D1(25) = 0.0
D1(26) = 0.0
D1(27) = 0.0
D1(28) = 0.1445164821E-08
D1(29) = 0.0
D1(30) = 0.9915173756E-09
```

ROTATION METHOD FOR A MOLECULE WITH K = -0.5,
WITHOUT A TENDENCY

```
nonreduced - S
T( 1) = 0.1751825970E-05
T( 2) =-0.1204722699E-04
T( 3) = 0.1212737623E-04
T( 4) =-0.1317521411E-06
T( 5) = 0.1777054318E-05
T( 6) =-0.1645447950E-05
T( 7) =-0.1338756416E-06
T( 8) = 0.2376071965E-05
T( 9) =-0.5275868803E-07
T(10) =-0.3101449613E-05
T(11) =-0.2242969070E-05
T(12) = 0.3154869389E-05
D( 1) =-0.2356707353E-01
D( 2) =-0.2790831301E+00
D( 3) =-0.1621607474E-02
D( 4) = 0.1000000000E-04

D1( 1) =-0.2356606800E-01
D1( 2) =-0.2790866214E+00
D1( 3) =-0.1581357543E-02
D1( 4) = 0.9489857629E-05
```

```
D( 5) = 0.1000000000E-04      D1( 5) =-0.4798223019E-03
D( 6) = 0.1000000000E-04      D1( 6) = 0.0
D( 7) = 0.1000000000E-04      D1( 7) = 0.9993246730E-03
D( 8) = 0.1000000000E-04      D1( 8) = 0.9256259239E-06
D( 9) = 0.1000000000E-04      D1( 9) = 0.0
D(10) = 0.1000000000E-04      D1(10) = 0.2997689935E-04
D(11) = 0.1000000000E-04      D1(11) = 0.0
D(12) = 0.1000000000E-04      D1(12) = 0.1026725271E-04
D(13) = 0.1000000000E-08      D1(13) = 0.4818470771E-08
D(14) = 0.1000000000E-08      D1(14) = 0.4234562220E-04
D(15) = 0.1000000000E-08      D1(15) = 0.0
D(16) = 0.1000000000E-08      D1(16) =-0.8469030236E-04
D(17) = 0.1000000000E-08      D1(17) =-0.1084036836E-03
D(18) = 0.1000000000E-08      D1(18) = 0.0
D(19) = 0.1000000000E-08      D1(19) = 0.6637581836E-08
D(20) = 0.1000000000E-08      D1(20) = 0.0
D(21) = 0.1000000000E-08      D1(21) = 0.0
D(22) = 0.1000000000E-08      D1(22) = 0.2167599501E-03
D(23) = 0.1000000000E-08      D1(23) = 0.4965667823E-07
D(24) = 0.1000000000E-08      D1(24) = 0.0
D(25) = 0.1000000000E-08      D1(25) = 0.0
D(26) = 0.1000000000E-08      D1(26) = 0.0
D(27) = 0.1000000000E-08      D1(27) = 0.0
D(28) = 0.1000000000E-08      D1(28) = 0.1090764615E-08
D(29) = 0.1000000000E-08      D1(29) = 0.0
D(30) = 0.1000000000E-08      D1(30) =-0.2637581836E-08

nonreduced - A
T( 1) =-0.5978878433E-04
T( 2) = 0.1223718247E-03
T( 3) =-0.7351092316E-04
T( 4) = 0.2020385891E-05
T( 5) =-0.2995324765E-04
T( 6) = 0.2765682226E-04
T( 7) = 0.2376481188E-05
T( 8) =-0.3975792084E-04
T( 9) =-0.1199596473E-04
T(10) = 0.1166138269E-03
T(11) = 0.3764884875E-04
T(12) =-0.1187205386E-03
D( 1) =-0.2356707353E-01      D1( 1) =-0.2360682059E-01
D( 2) =-0.2790831301E+00      D1( 2) =-0.2789250579E+00
D( 3) =-0.1621607474E-02      D1( 3) =-0.3925987866E-02
D( 4) = 0.1000000000E-04      D1( 4) = 0.3007280778E-04
D( 5) = 0.1000000000E-04      D1( 5) = 0.1008520053E-01
D( 6) = 0.1000000000E-04      D1( 6) = 0.0
D( 7) = 0.1000000000E-04      D1( 7) =-0.2038065376E-01
D( 8) = 0.1000000000E-04      D1( 8) = 0.2817751862E-03
D( 9) = 0.1000000000E-04      D1( 9) = 0.0
D(10) = 0.1000000000E-04      D1(10) = 0.2999800000E-04
D(11) = 0.1000000000E-04      D1(11) = 0.9831173908E-03
D(12) = 0.1000000000E-04      D1(12) = 0.0
D(13) = 0.1000000000E-08      D1(13) =-0.1940389196E-07
D(14) = 0.1000000000E-08      D1(14) =-0.7069910302E-03
```

```
D(15) = 0.1000000000E-08
D(16) = 0.1000000000E-08
D(17) = 0.1000000000E-08
D(18) = 0.1000000000E-08
D(19) = 0.1000000000E-08
D(20) = 0.1000000000E-08
D(21) = 0.1000000000E-08
D(22) = 0.1000000000E-08
D(23) = 0.1000000000E-08
D(24) = 0.1000000000E-08
D(25) = 0.1000000000E-08
D(26) = 0.1000000000E-08
D(27) = 0.1000000000E-08
D(28) = 0.1000000000E-08
D(29) = 0.1000000000E-08
D(30) = 0.1000000000E-08
```

```
D1(15) = 0.0
D1(16) = 0.1428206751E-02
D1(17) = 0.3176993233E-02
D1(18) = 0.0
D1(19) = 0.4000000000E-08
D1(20) = 0.0
D1(21) = 0.6600972989E-08
D1(22) =-0.6401083044E-02
D1(23) = 0.3289929142E-04
D1(24) = 0.0
D1(25) = 0.0
D1(26) = 0.1850769775E-03
D1(27) = 0.0
D1(28) = 0.0
D1(29) = 0.0
D1(30) = 0.0
```

```
A - S
T( 1) = 0.6151052744E-04
T( 2) =-0.1343133769E-03
T( 3) = 0.8554071179E-04
T( 4) =-0.2151062855E-05
T( 5) = 0.3171577464E-04
T( 6) =-0.2928881164E-04
T( 7) =-0.2509257913E-05
T( 8) = 0.4211456770E-04
T( 9) = 0.1194363432E-04
T(10) =-0.1196899568E-03
T(11) =-0.3987348141E-04
T(12) = 0.1218496567E-03
D( 1) =-0.2360682059E-01
D( 2) =-0.2789250579E+00
D( 3) =-0.3925987866E-02
D( 4) = 0.3007280778E-04
D( 5) = 0.1008520053E-01
D( 6) = 0.0
D( 7) =-0.2038065376E-01
D( 8) = 0.2817751862E-03
D( 9) = 0.0
D(10) = 0.2999800000E-04
D(11) = 0.9831173908E-03
D(12) = 0.0
D(13) =-0.1940389196E-07
D(14) =-0.7069910302E-03
D(15) = 0.0
D(16) = 0.1428206751E-02
D(17) = 0.3176993233E-02
D(18) = 0.0
D(19) = 0.4000000000E-08
D(20) = 0.0
D(21) = 0.6600972989E-08
D(22) =-0.6401083044E-02
D(23) = 0.3289929142E-04
D(24) = 0.0
```

```
D1( 1) =-0.2356624692E-01
D1( 2) =-0.2790862203E+00
D1( 3) =-0.1581902744E-02
D1( 4) = 0.9354659182E-05
D1( 5) =-0.4758152278E-03
D1( 6) = 0.0
D1( 7) = 0.9912401116E-03
D1( 8) = 0.1130079136E-05
D1( 9) = 0.0
D1(10) = 0.2997725000E-04
D1(11) = 0.0
D1(12) = 0.1033489873E-04
D1(13) = 0.4771680660E-08
D1(14) = 0.4199940727E-04
D1(15) = 0.0
D1(16) =-0.8399784392E-04
D1(17) =-0.1075180850E-03
D1(18) = 0.0
D1(19) = 0.6593750229E-08
D1(20) = 0.0
D1(21) = 0.0
D1(22) = 0.2149893594E-03
D1(23) = 0.4906829661E-07
D1(24) = 0.0
```

```
D(25) = 0.0                    D1(25) = 0.0
D(26) = 0.1850769775E-03       D1(26) = 0.0
D(27) = 0.0                    D1(27) = 0.0
D(28) = 0.0                    D1(28) = 0.1114159670E-08
D(29) = 0.0                    D1(29) = 0.0
D(30) = 0.0                    D1(30) =-0.2593750229E-08
```

APPENDIX E

A-A FITTING FOR TRUNCATED NH_2 SPECTRUM

Source	Number	Std. Dev.	Scaled
MODR	31	0.2027 MHz	0.6757
LMR	24	0.0004 Cm-1	1.0698
ABS	5694	0.0137 Cm-1	0.9147
EMS	12	0.0214 Cm-1	0.7123
All	5761	3.7472 MHz	0.9165
Ratio	Cm-1	Std. Dev.	
0.0000	1.31307157E+01	7.79729421E-05	A-K
0.0000	1.05623424E+01	3.23549439E-05	A-N
0.0000	1.19478656E+00	1.48926715E-05	a
0.0006	-2.20112098E-02	1.31265168E-05	D-KK
0.0018	4.19109153E-03	7.44388906E-06	D-KN
0.0012	-1.05537991E-03	1.24332401E-06	D-NN
0.0061	-1.00795326E-03	6.16377885E-06	d-K
0.0014	-4.22893123E-04	5.89370589E-07	d-N
0.0103	6.98173065E-05	7.15760636E-07	H-KKK
0.0388	-1.47006286E-05	5.69968436E-07	H-KKN
0.4888	-3.74943973E-07	1.83276440E-07	H-KNN
0.0313	4.07699366E-07	1.27678452E-08	H-NNN
0.0371	2.02883929E-05	7.51811362E-07	h-KK
0.1976	-4.75440648E-07	9.39517418E-08	h-KN
0.0273	2.06125302E-07	5.61982019E-09	h-NN
0.0478	-2.62535989E-07	1.25531927E-08	L-KKKK
0.1579	3.99714867E-08	6.31282917E-09	L-KKKN
0.3094	-4.48294993E-08	1.38685967E-08	l-KKK
0.0929	5.95831036E-10	5.53566193E-11	J(Z)**10
0.0001	-2.86721832E-01	1.52328348E-05	(S)A-K
0.0001	-2.23874909E-02	3.02062351E-06	(S)A-N
0.0002	-1.14045492E-02	2.82726284E-06	(S)a'
0.0073	1.11779483E-03	8.15979262E-06	(S)D-KK
0.0985	-9.65366176E-05	9.50533600E-06	(S)D-KN
0.3993	-2.29953084E-05	9.18281167E-06	(S)D-NK
0.0205	1.11770735E-05	2.29351467E-07	(S)D-NN
0.0827	2.60196393E-05	2.15265009E-06	(S)d-K
0.0219	5.56548018E-06	1.21843445E-07	(S)d-N
0.1483	-4.09702244E-06	6.07543288E-07	(S)H-KKK
0.3796	1.26038351E-06	4.78479820E-07	(S)H-KKN
0.3187	-1.50741541E-08	4.80468553E-09	(S)H-NNN
0.3703	-7.20992926E-07	2.67019609E-07	(S)h-KK
0.3055	-8.46801868E-09	2.58679329E-09	(S)h-NN

S-S FITTING FOR TRUNCATED NH_2 SPECTRUM

Source	Number	Std. Dev.	Scaled
MODR	31	0.2304 MHz	0.7680
LMR	24	0.0004 Cm-1	1.1007
ABS	5694	0.0137 Cm-1	0.9146
EMS	12	0.0218 Cm-1	0.7275
All	5761	3.7482 MHz	0.9168

Ratio	Cm-1	Std. Dev.	
0.0000	1.31312536E+01	7.31488345E-05	A-K
0.0000	1.05622147E+01	3.03443816E-05	A-N
0.0000	1.19379786E+00	1.44610014E-05	a
0.0006	-2.16540994E-02	1.25251274E-05	D-KK
0.0014	3.73666713E-03	5.40708809E-06	D-KN
0.0010	-9.77548681E-04	9.48615550E-07	D-NN
0.0013	-4.23204978E-04	5.61867383E-07	d-N
0.0056	-3.95078024E-05	2.21562194E-07	d
0.0090	5.95344963E-05	5.35082098E-07	H-KKK
0.0153	-4.58878706E-06	7.02148920E-08	H-KNN
0.0211	3.82912442E-07	8.07017458E-09	H-NNN
0.0314	1.61202815E-07	5.06333289E-09	h-NN
0.1970	1.80675394E-08	3.55977963E-09	h-N
0.0316	4.83410442E-08	1.52982632E-09	h
0.0378	-2.63362266E-07	9.95509246E-09	L-KKKK
0.0548	3.75570173E-08	2.05884907E-09	L-KKKN
0.0886	6.13323902E-10	5.43496314E-11	J(Z)**10
0.0000	-2.86741741E-01	1.26237132E-05	(S)A-K
0.0001	-2.23824450E-02	2.76778103E-06	(S)A-N
0.0001	-1.13771584E-02	1.58877083E-06	(S)a'
0.0048	1.10636091E-03	5.28782492E-06	(S)D-KK
0.1327	-6.17940390E-05	8.20270515E-06	(S)D-KN
0.1750	-4.64482540E-05	8.13075604E-06	(S)D-NK
0.0111	9.67277484E-06	1.07799863E-07	(S)D-NN
0.0106	5.26759210E-06	5.58512003E-08	(S)d-N
0.1676	3.79049377E-07	6.35348879E-08	(S)d'
0.1320	-3.40909262E-06	4.50151048E-07	(S)H-KKK
0.3950	6.32977756E-07	2.50012938E-07	(S)H-KKN
0.4947	4.11812777E-09	2.03703728E-09	(S)h-N
0.3491	6.48074709E-09	2.26236377E-09	(S)h'

A-A FITTING FOR COMPLETE NH_2 SPECTRUM

Source	Number	Std. Dev.	Scaled
MODR	31	0.2750 MHz	0.9168
LMR	24	0.0006 Cm-1	1.4690
ABS	5694	0.0139 Cm-1	0.9237
EMS	44	0.0465 Cm-1	1.5497
All	5793	3.8380 MHz	0.9361

Ratio	Cm-1	Std. Dev.	
0.0000	1.31301871E+01	4.44593974E-05	A-K
0.0000	1.05622514E+01	4.36974657E-05	A-N
0.0000	1.19483222E+00	2.05837767E-05	a
0.0004	-2.19020192E-02	8.89892070E-06	D-KK
0.0015	4.17364330E-03	6.38660914E-06	D-KN
0.0016	-1.05119144E-03	1.68554866E-06	D-NN
0.0132	-1.01405461E-03	1.34328886E-05	d-K
0.0020	-4.24042432E-04	8.28279292E-07	d-N
0.0224	6.10370225E-05	1.36987827E-06	H-KKK
0.1990	-9.54090150E-06	1.89832540E-06	H-KKN
0.4008	-1.40413542E-06	5.62841644E-07	H-KNN
0.0462	3.64208525E-07	1.68319000E-08	H-NNN
0.0782	1.89768260E-05	1.48458564E-06	h-KK

0.7462	-3.59544888E-07	2.68288618E-07	h-KN
0.0422	2.16551600E-07	9.13879061E-09	h-NN
0.0631	-2.92684598E-07	1.84675043E-08	L-KKKK
0.1784	2.36137375E-07	4.21195684E-08	L-KKKN
0.2525	-1.16829351E-07	2.94969788E-08	L-KKNN
0.3533	1.66388149E-08	5.87850627E-09	L-KNNN
0.1434	-1.44945769E-07	2.07840880E-08	l-KKK
0.4919	4.26180161E-08	2.09633830E-08	l-KKN
0.5093	-3.58657523E-09	1.82673366E-09	l-KNN
0.0124	3.36517690E-10	4.18548124E-12	J(Z)**10
0.0195	-3.28618821E-13	6.39765604E-15	J(Z)**12
0.0001	-2.86703751E-01	1.47686059E-05	(S)A-K
0.0001	-2.23959005E-02	3.34528072E-06	(S)A-N
0.0009	-1.14793914E-02	1.08493246E-05	(S)a'
0.0067	1.10403064E-03	7.36682585E-06	(S)D-KK
0.0897	-1.41703135E-04	1.27065838E-05	(S)D-KN
0.4975	2.57045180E-05	1.27891180E-05	(S)D-NK
0.0298	1.31896339E-05	3.93514391E-07	(S)D-NN
0.1056	1.04856311E-04	1.10773066E-05	(S)d-K
0.0347	6.89029582E-06	2.38975042E-07	(S)d-N
0.1250	-8.09529400E-06	1.01179237E-06	(S)H-KKK
0.1527	8.32221049E-06	1.27068806E-06	(S)H-KKN
0.1402	-2.13198910E-06	2.98806733E-07	(S)H-KNN
0.1362	-8.71292194E-08	1.18689239E-08	(S)H-NNN
0.1321	-1.01189181E-05	1.33683955E-06	(S)h-KK
0.1767	-4.11490777E-07	7.27123751E-08	(S)h-KN
0.1363	-5.50275091E-08	7.49950298E-09	(S)h-NN

S-S FITTING FOR THE COMPLETE NH_2 SPECTRUM

Source	Number	Std. Dev.	Scaled
MODR	31	0.2686 MHz	0.8954
LMR	24	0.0006 Cm-1	1.5486
ABS	5694	0.0139 Cm-1	0.9293
EMS	44	0.0590 Cm-1	1.9661
All	5793	3.8850 MHz	0.9476
Ratio	Cm-1	Std. Dev.	
0.0000	1.31308869E+01	4.11742814E-05	A-K
0.0000	1.05620874E+01	3.82411578E-05	A-N
0.0000	1.19381770E+00	1.49070108E-05	a
0.0003	-2.15264989E-02	7.36448912E-06	D-KK
0.0013	3.69335210E-03	4.67413229E-06	D-KN
0.0016	-9.68034616E-04	1.50686236E-06	D-NN
0.0014	-4.22398326E-04	5.99348757E-07	d-N
0.0057	-4.06919664E-05	2.33710543E-07	d
0.0048	5.14809909E-05	2.45463219E-07	H-KKK
0.0962	3.99183106E-06	3.84019024E-07	H-KKN
0.0327	-5.22291171E-06	1.70683048E-07	H-KNN
0.0546	2.83776082E-07	1.54841996E-08	H-NNN
0.0378	1.46758650E-07	5.55114644E-09	h-NN
0.1215	3.18701479E-08	3.87211840E-09	h-N
0.0352	4.75438815E-08	1.67396200E-09	h
0.0223	-1.72721204E-07	3.85166820E-09	L-KKKK
0.2200	4.07056835E-08	8.95545116E-09	L-KKKN

0.2330	-3.27778059E-08	7.63797500E-09	L-KKNN
0.1965	1.16727754E-08	2.29319832E-09	L-KNNN
0.0121	3.12577708E-10	3.77864237E-12	J(Z)**10
0.0168	-2.81346651E-13	4.72685537E-15	J(Z)**12
0.0000	-2.86729384E-01	1.28447400E-05	(S)A-K
0.0001	-2.23885271E-02	2.69963644E-06	(S)A-N
0.0002	-1.13803996E-02	2.02254997E-06	(S)a'
0.0046	1.10169890E-03	5.04456935E-06	(S)D-KK
0.1347	-6.31622619E-05	8.50484838E-06	(S)D-KN
0.2109	-4.13144176E-05	8.71464952E-06	(S)D-NK
0.0106	9.96363662E-06	1.05698553E-07	(S)D-NN
0.0231	5.60930401E-06	1.29606541E-07	(S)d-N
0.1890	6.99455272E-07	1.32180077E-07	(S)d'
0.4082	-7.99842396E-07	3.26532265E-07	(S)H-KKK
0.3422	-8.88006725E-07	3.03867619E-07	(S)H-KNK
0.3504	-6.80738450E-09	2.38563196E-09	(S)h-NN
0.4367	-1.18410754E-08	5.17118157E-09	(S)h-N
0.6229	-7.13701277E-09	4.44576635E-09	(S)h'